Fig. 1

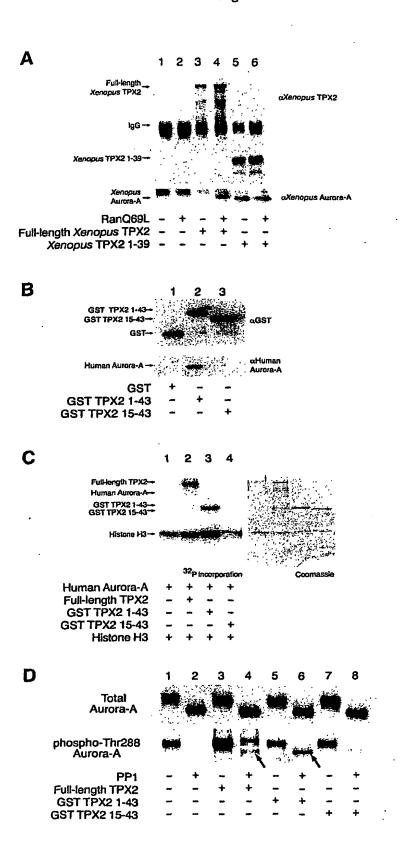
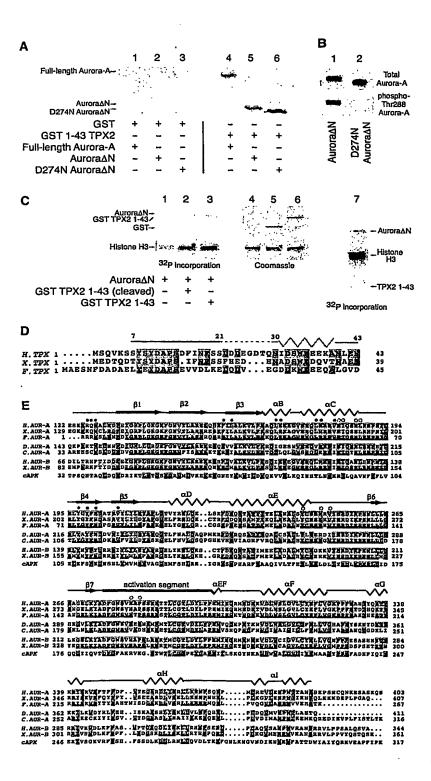


Fig. 2





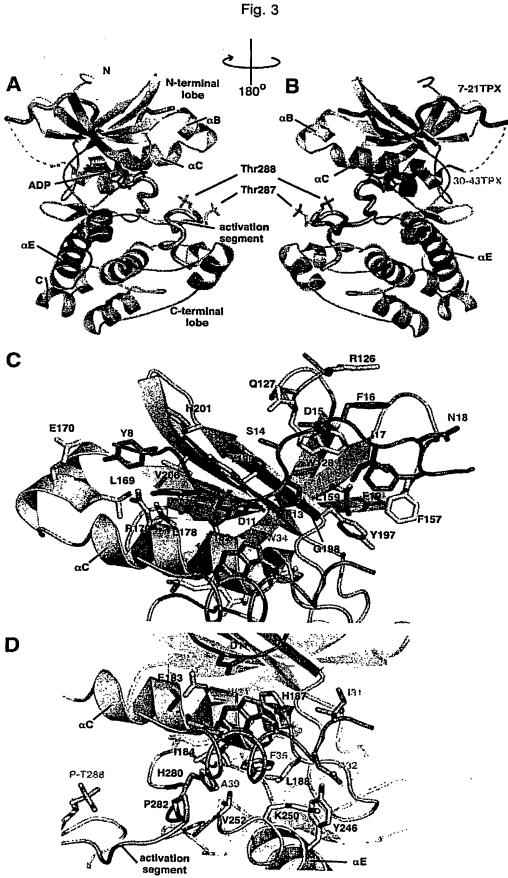
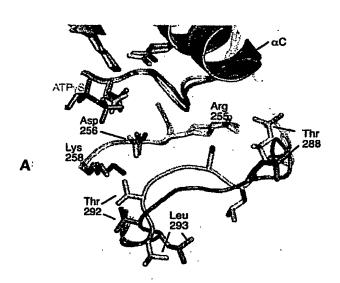


Fig. 4



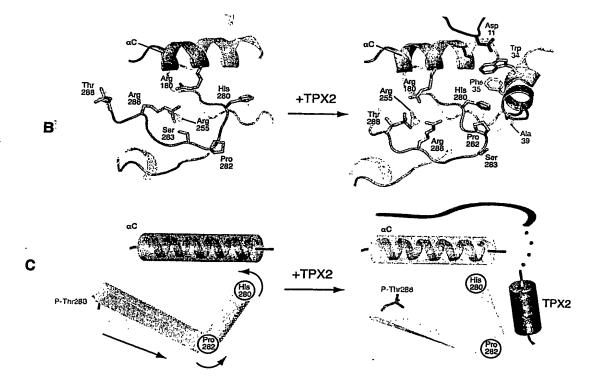


Fig. 5

| т | ٠, | h | Λ |
|-----|----|---|--------|
| - 1 | а | מ | \sim |

| ATOM | 1 | CB | GLN A | 127 | 267.519 | ~61.189 | 87.734 | 1.00 | 66.58 | F | A C |
|------|----|-----|-------|-----|----------|---------|---------|--------|-------|------------|-----|
| ATOM | 2 | CG | GLN A | 127 | 266, 971 | -61.391 | 86.330 | 1.00 | | I | |
| MOTA | 3 | CD | GLN A | | | -60.121 | 85.741 | 1.00 | | | |
| | 4 | | GLN A | | | | | | | Į | |
| ATOM | _ | | | | | -60.183 | 84.781 | 1.00 | | P | |
| MOTA | 5 | | GLN A | | | -58.962 | 86.307 | 1.00 | | F | |
| ATOM | 6 | C | GLN A | 127 | 269.192 | -59.883 | 89.051 | 1.00 | 63.35 | F | A C |
| MOTA | 7 | 0 | GLN A | 127 | 269.877 | ~58.853 | 89.024 | 1.00 | 70.04 | Į | A 0 |
| MOTA | 8 | N | GLN A | 127 | 269,910 | -61.949 | 87.808 | 1.00 | 58.04 | F | |
| ATOM | 9 | CA | GLN A | 127 | | -60.755 | 87.810 | 1.00 | | | A C |
| ATOM | 10 | N | TRP A | | | -60.307 | 90.137 | 1.00 | | | |
| ATOM | 11 | CA | TRP A | | | -59.552 | 91.366 | | | F | |
| | | | | | | | | 1.00 | | | 7 C |
| ATOM | 12 | CB | TRP A | | | -59.733 | 92.133 | 1.00 | | F | 7 C |
| MOTA | 13 | CG | TRP A | | | -59.256 | 91.369 | 1.00 | | F | |
| MOTA | 14 | | TRP A | | | -57.928 | 90.897 | 1.00 | 50.34 | P | A C |
| ATOM | 15 | CE2 | TRP A | 128 | 264.697 | -57.962 | 90.150 | 1.00 | 53.33 | P | A C |
| MOTA | 16 | CE3 | TRP A | 128 | 266.611 | -56.713 | 91.017 | 1.00 | 53.44 | P | Y C |
| ATOM | 17 | CD1 | TRP A | 128 | 265.096 | -60.014 | 90.921 | 1.00 | | F | |
| MOTA | 18 | NE1 | TRP A | 128 | 264.228 | -59.249 | 90.191 | 1.00 | | F | |
| ATOM | 19 | | TRP A | | | -56.816 | 89.514 | 1.00 | | 7 | |
| ATOM | 20 | | TRP A | | | -55.571 | 90.392 | | | | |
| | | | TRP A | | | | | 1.00 | | P | |
| MOTA | 21 | | | | | -55.633 | 89.639 | 1.00 | | P | |
| MOTA | 22 | C | TRP A | | | -59.909 | 92.262 | 1.00 | | P | Y C |
| ATOM | 23 | 0 | TRP A | | | -61.026 | 92.231 | 1.00 | 54.76 | P | • 0 |
| ATOM | 24 | N | ALA A | 129 | 270.184 | -58.955 | 93.085 | 1.00 | 55.48 | P | N A |
| MOTA | 25 | CA | ALA A | 129 | 271.283 | -59.206 | 94.006 | 1.00 | 60.01 | P | C |
| ATOM | 26 | CB | ALA A | 129 | 272.608 | -58.800 | 93.341 | 1.00 | | 7 | |
| ATOM | 27 | С | ALA A | 129 | | -58.371 | 95.258 | 1.00 | | P | _ |
| ATOM | 28 | . 0 | ALA A | | | -57.326 | 95.173 | 1.00 | | ZA | |
| ATOM | 29 | N | LEU A | | | -58.821 | | | | | |
| | 30 | CA | LEU A | | | | 96.401 | 1.00 | | A | |
| ATOM | | | | | | -58.126 | 97.665 | 1.00 | | A | |
| ATOM | 31 | CB | LEU A | | | -58.770 | 98.787 | 1.00 | | P | , C |
| MOTA | 32 | CG | LEU A | | | -58.110 | | 1.00 | 36.68 | A | C |
| ATOM | 33 | | LEU A | | | -57.934 | | 1.00 | 47.13 | A | C |
| ATOM | 34 | CD2 | LEU A | 130 | 272.839 | -58.975 | 101.186 | 1.00 | 38.64 | 2 A | C |
| ATOM | 35 | C | LEU A | 130 | 271.750 | -56.702 | 97.591 | 1.00 5 | 55.17 | A | |
| MOTA | 36 | 0 | LEU A | 130 | 271.223 | -55.834 | 98.305 | 1.00 | | A | |
| ATOM | 37 | N | GLU A | 131 | | -56.469 | 96.690 | 1.00 | | A | |
| ATOM | 38 | CA | GLU A | | | -55.172 | 96.539 | 1.00 | | A | |
| ATOM | 39 | CB | GLU A | | | -55.400 | 96.030 | 1.00 | | | |
| | 40 | CG | | | | | | | | A | |
| MOTA | | | GLU A | | | -56.450 | 96.938 | 1.00 | | A | |
| ATOM | 41 | CD | GLU A | | | -57.909 | 96.486 | 1.00 | | A | |
| ATOM | 42 | | GLU A | | | -58.142 | 95.477 | 1.00 8 | 30.97 | A | . 0 |
| ATOM | 43 | | GLU A | | 275.838 | -58.820 | 97.135 | 1.00 8 | 38.53 | A | . 0 |
| MOTA | 44 | С | GLU A | 131 | 272.458 | -54.235 | 95.682 | 1.00 5 | 35.07 | A | . c |
| ATOM | 45 | 0 | GLU A | 131 | 272.851 | -53.119 | 95.439 | 1.00 5 | 51.83 | A | . 0 |
| ATOM | 46 | N | ASP A | 132 | 271.280 | -54.704 | 95.299 | 1.00 5 | 33.60 | А | |
| ATOM | 47 | CA | ASP A | 132 | 270.298 | ~53.994 | 94.487 | 1.00 5 | | A | |
| ATOM | 48 | CB | ASP A | 132 | 269.514 | -54.987 | 93.656 | 1.00 | | A | |
| ATOM | 49 | CG | ASP A | | | -55.141 | 92.284 | 1.00 | | | |
| ATOM | 50 | | ASP A | | | -54.250 | | | | A | |
| | 51 | | ASP A | | | | 91.447 | 1.00 7 | | A | |
| ATOM | | | | | | -56.159 | 92.048 | 1.00 7 | | A | |
| ATOM | 52 | С | ASP A | | | -53.412 | 95.449 | 1.00 5 | | A | C |
| ATOM | 53 | 0 | ASP A | | | -52.547 | 95.093 | 1.00 5 | 6.43 | A | . 0 |
| ATOM | 54 | N | PHE A | | 269.239 | -53.925 | 96.666 | 1.00 € | 52.15 | A | N |
| ATOM | 55 | CA | PHE A | 133 | 268.239 | -53.448 | 97.598 | 1.00 6 | 52.91 | A | С |
| ATOM | 56 | CB | PHE A | 133 | 267.324 | -54.622 | 97.974 | 1.00 5 | | A | |
| ATOM | 57 | CG | PHE A | | | -55.337 | 96.775 | 1.00 6 | | A | |
| ATOM | 58 | | PHE A | | | -56.312 | 96.095 | 1.00 6 | | A | |
| ATOM | 59 | | PHE A | | | -55.059 | 96.346 | 1.00 6 | | | |
| ATOM | 60 | | PHE A | | | -56.996 | | | | A | |
| ATOM | 61 | | PHE A | | | | 94.991 | 1.00 € | | A | |
| | | | | | | -55.719 | 95.264 | 1.00 6 | | A | |
| MOTA | 62 | CZ | PHE A | 133 | 205.607 | -56.697 | 94.585 | 1.00 6 | 1.32 | Α | C |
| | | | | | | | | | | | |

| ATOM | 63 | С | PHE A 1 | | 268.740 | -52.733 | 98.847 | | 61.07 | P | | С |
|--------------|------------|----------|--------------------|------|--------------------|--------------------|--------------------|------|----------------|--------|--------------|--------|
| ATOM | 64 | 0 | PHE A 1 | | 269.866 | | 99.318 | | 66.24 | P | | 0 |
| ATOM | 65 | N | GLU A 1 | | 267.878 | | 99.340 | | 59.55 | F | | N |
| ATOM | 66 | CA | GLU A 1 | | 268.062 267.589 | | | | 58.90 54.77 | P P | | C |
| ATOM | 67 68 | CB CG | GLU A 1 | | 268.478 | | 99.488 | | 63.45 | F | | c |
| ATOM ATOM | 69 | CD | GLU A 1 | | 268.205 | | 99.556 | | 61.84 | Į | | č |
| ATOM | 70 | | GLU A 1 | | 268.808 | | | | 75.06 | I | | 0 |
| ATOM | 71 | | GLU A 1 | | 267.388 | | 98.768 | 1.00 | 73.27 | 7 | Į. | 0 |
| ATOM | 72 | C - | GLU A 1 | 34 | 267.139 | -51.698 | 101.627 | 1.00 | 53.85 | Į | 7 | С |
| ATOM | 73 | 0 | GLU A 1 | 34 | 265.909 | | | | 60.03 | | j | 0 |
| ATOM | 74 | N | ILE A 1 | | 267.713 | - | | | 52.32 | | 4 | N |
| MOTA | 75 | CA | ILE A 1 | | 266.917 | | | | 50.89 | | Ä | C |
| ATOM | 76 | CB | ILE A 1 | | 267.750 | -54.131 | | | 48.23 | |) | C |
| ATOM | 77 | | ILE A 1 ILE A 1 | | | -54.940 | | | 48.00 | | | C |
| ATOM | 78 79 | | ILE A 1 | | | -55.720 | | | 35.46 | | À | c |
| ATOM ATOM | 80 | CDI | ILE A 1 | | | -52.129 | | | 50.54 | | Ā | Ċ |
| MOTA | 81 | ŏ | ILE A 1 | | | -51.281 | | | 50.32 | | A | 0 |
| ATOM | 82 | N | GLY A 1 | | 265.004 | -52.334 | 104.924 | 1.00 | 49.85 | 1 | Ą | N |
| ATOM | 83 | CA | GLY A 1 | .36 | 264.286 | -51.534 | 105.903 | 1.00 | 44.78 | 1 | A | С |
| MOTA | 84 | C | GLY A 1 | .36 | | -52.255 | | | 44.85 | | Ą | С |
| MOTA | 85 | 0 | GLY A 1 | | | -53.071 | | | 45.10 | | A. | 0 |
| MOTA | 86 | N | ARG A 1 | | | -51.996 | | | 40.54 | | A. | N |
| ATOM | 87 | CA | ARG A 1 | | | -52.598 | | | 47.22 46.15 | | A. | C |
| MOTA | 88 | CB | ARG A 1 | | | -51.766 -51.887 | | | 46.13 | | A A | C |
| ATOM | 89 90 | CG CD | ARG A 1 | | | -51.284 | | | 47.76 | | A. | č |
| ATOM ATOM | 91 | NE | ARG A 1 | | | -51.283 | | | 44.18 | | A. | N |
| ATOM | 92 | CZ | ARG A 1 | | | -52.330 | | | 49.13 | | A | С |
| ATOM | 93 | | ARG A 1 | | | | 110.655 | 1.00 | 50.41 | | A | N |
| ATOM | 94 | NH2 | ARG A 1 | 1.37 | 256.144 | -52.230 | 109.579 | 1.00 | 42.98 | 1 | A | N |
| MOTA | 95 | С | ARG A 1 | L37 | | -54.014 | | | 48.40 | | A. | С |
| ATOM | 96 | 0 | ARG A 1 | | | -54.370 | | | 52.53 | | A | 0 |
| MOTA | 97 | N | PRO A 1 | | | -54.840 | | | 48.54 | | A | И С |
| ATOM | 98 | CD | PRO A 1 | | | ~54.581 ~56.226 | | 1.00 | 46.06 46.02 | | A A | c |
| MOTA | 99 100 | CA CB | PRO A 1 | | | -56.765 | | | 49.55 | | A. | c |
| MOTA MOTA | 101 | CG | PRO A | | | -55.955 | | | 42.97 | | A | Ċ |
| ATOM | 102 | Ċ | PRO A | | | -56.262 | | | 49.85 | | A | С |
| MOTA | 103 | 0 | PRO A | 138 | 259.920 | -55.810 | 111.142 | 1.00 | 50.42 | | A | 0 |
| ATOM | 104 | N | LEU A | 139 | | | 109.138 | | 45.75 | | A | N |
| MOTA | 105 | CA | LEU A | | | | 109.005 | | 39.58 | | A | C |
| MOTA | 106 | CB | LEU A | | | | 107.558 | | 37.24 | | A 7 | C |
| ATOM | 107 | CG | LEU A | | | | 106.664 105.170 | | 42.68 | | A A | C |
| MOTA | 108 109 | | LEU A : | | | | 103.170 | | 43.77 | | A | c |
| MOTA MOTA | 110 | C | LEU A | | | | 109.880 | | 40.81 | | A | Č |
| ATOM | 111 | ō | LEU A | | | | 110.480 | | 45.92 | | A | 0 |
| ATOM | 112 | N | GLY A | | 258.675 | -59.111 | 109.970 | 1.00 | 45.15 | | Ά | N |
| ATOM | 113 | CA | GLY A | 140 | - | | 110.789 | | 48.82 | | A | С |
| MOTA | 114 | С | GLY A | | | | 111.040 | | 48.37 | | A | C |
| ATOM | 115 | 0 | GLY A | | | | 110.492 | | 53.08 | | A. | 0 |
| MOTA | 116 | N | LYS A | | | | 111.856 112.192 | | 52.66 56.79 | | A A | N C |
| ATOM | 117 | CA | LYS A : | | | | 113.707 | | 61.89 | | A | c |
| ATOM ATOM | 118 119 | CB CG | LYS A | | | | 114.210 | | 68.25 | | A | C |
| ATOM | 120 | CD | LYS A | | | | 115.750 | | 78.79 | | A | Ċ |
| ATOM | 121 | CE | LYS A | | | | 116.242 | | 83.42 | | A | С |
| ATOM | 122 | NZ | LYS A | 141 | 261.987 | -65.651 | 117.745 | 1.00 | 90.84 | | A | N |
| MOTA | 123 | С | LYS A | | | | 111.704 | | 57.82 | | A | С |
| ATOM | 124 | 0 | LYS A | | | | 112.084 | | 57.17 | | A | 0 |
| MOTA | 125 | N | GLY A | | | | 110.823 | | 63.79 | | A 7 | N |
| ATOM | 126 | CA | GLY A | | | | 110.315 111.087 | | 67.77 | | A | C C |
| MOTA | 127 | C | GLY A | | | | 111.087 | | 68.12 76.19 | | A A | 0 |
| ATOM | 128 129 | N N | GLY A : | | | | 110.410 | | 66.29 | | A | И |
| MOTA MOTA | 130 | CA | LYS A | | | | 111.016 | | 62.91 | | A | Ċ |
| ATOM | 131 | CB | LYS A | | 260.576 | -71.221 | 110.783 | | 56.50 | | A | Ċ |
| ATOM | 132 | CG | LYS A | | | | 111.694 | | 59.59 | | A | С |

| ATOM | 133 | CD | LYS | A | 143 | 259.804 | -73.170 | 112.130 | 1.00 | 65.95 | A | С |
|--------------|------------|----------|-----|---|------------|---------|--------------------|---------|------|----------------|--------|--------|
| ATOM | 134 | CE | LYS | A | 143 | | -74.141 | | 1.00 | 69.37 | A | С |
| MOTA | 135 | NZ | LYS | Α | 143 | 259.069 | -75.109 | 113.596 | 1.00 | 70.95 | A | N |
| MOTA | 136 | С | LYS | Α | 143 | 262.773 | -70.081 | 110.500 | 1.00 | 62.52 | A | С |
| MOTA | 137 | 0 | LYS | Α | 143 | 263.725 | -70.302 | 111.243 | 1.00 | 61.60 | A | 0 |
| ATOM | 138 | N | PHE | Α | 144 | | -69.898 | | 1.00 | 68.60 | A | N |
| ATOM | 139 | CA | PHE | Α | 144 | 264.215 | -70.021 | 108.556 | 1.00 | 74.62 | A | С |
| MOTA | 140 | CB | PHE | | | | -70.886 | | 1.00 | 69.32 | A | С |
| ATOM | 141 | CG | PHE | | | | -72.278 | | | 69.58 | A | С |
| ATOM | 142 | | PHE | | | | -72.526 | | | 66.23 | A | С |
| ATOM | 143 | | PHE | | | | -73.335 | | | 63.51 | A | C |
| MOTA | 144 | | PHE | | | | -73.816 | | | 73.24 | A | C |
| ATOM | 145 | | PHE | | | | -74.608 | | | 69.83 | A | C |
| ATOM | 146 | CZ | | | 144 | | -74.850 | | | 66.31 | A | C |
| ATOM | 147 148 | С 0 | | | 144 144 | | -68.665 -68.496 | | | 74.80 | A | C |
| ATOM ATOM | 149 | N | | | 145 | | -67.691 | | | 82.71 | A 7 | 0 |
| ATOM | 150 | CA | | | 145 | | -66.320 | | | 83.57 77.10 | A A | N C |
| ATOM | 151 | C | | | 145 | | -65.296 | | | 75.14 | A | c |
| ATOM | 152 | ŏ | | | 145 | | -65.557 | | | 74.64 | A | o |
| ATOM | 153 | N | | | 146 | | -64.097 | | | 67.46 | A | N |
| ATOM | 154 | CA | | | 146 | | -62.976 | | | 65.84 | A | C |
| ATOM | 155 | CB | | | 146 | | -61.895 | | | 68.52 | A | C |
| ATOM | 156 | CG | | | 146 | | -62.369 | | | 74.23 | A | c |
| ATOM | 157 | | ASN | A | 146 | | -63.577 | | | 76.10 | A | ō |
| ATOM | 158 | | ASN | | | | -61.415 | | | 74.93 | A | N |
| ATOM | 159 | C | ASN | Α | 146 | 262.727 | -62.402 | 107.955 | 1.00 | 60.10 | A | С |
| ATOM | 160 | 0 | ASN | Α | 146 | 263.442 | -62.661 | 106.979 | 1.00 | 60.40 | A | 0 |
| ATOM | 161 | N | VAL | Α | 147 | 261.651 | -61.614 | 107.909 | 1.00 | 49.34 | A | N |
| MOTA | 162 | CA | VAL | Α | 147 | 261.208 | -60.938 | 106.697 | 1.00 | 34.29 | A | С |
| ATOM | 163 | CB | VAL | Α | 147 | 259.691 | -61.195 | 106.433 | 1.00 | 35.55 | A | С |
| ATOM | 164 | CG1 | VAL | A | 147 | | -60.303 | | 1.00 | 22.76 | A | С |
| ATOM | 165 | CG2 | VAL | A | 147 | 259.444 | -62.657 | 106.040 | 1.00 | 25.36 | A | С |
| MOTA | 166 | С | VAL | Ą | 147 | | -59.427 | | 1.00 | 36.01 | A | С |
| ATOM | 167 | 0 | VAL | Α | 147 | 261.071 | -58.888 | 107.912 | 1.00 | 33.80 | A | 0 |
| MOTA | 168 | N | | | 148 | | -58.743 | | 1.00 | 38.73 | A | N |
| ATOM | 169 | CA | | | 148 | | -57.313 | | 1.00 | 38.16 | A | C |
| MOTA | 170 | CB | | | 148 | | -57.053 | | | 44.86 | A | С |
| ATOM | 171 | CG | | | 148 | | -57.783 | | | 51.34 | A | С |
| ATOM | 172 | CD1 | | | 148 | | -59.110 | | | 49.12 | A | С |
| ATOM | 173 | CE1 | | | 148 | | -59.799 | | | 57.49 | A | С |
| ATOM | 174 | | TYR | | | | -57.152 | | | 56.42 | A | C |
| ATOM ATOM | 175 176 | CE2 | | | 148 148 | | -57.839 -59.159 | | | 62.05 | A | C |
| ATOM | 177 | OH | | | 148 | | -59.818 | | | 59.22 | A | C |
| ATOM | 178 | C | | | 148 | | -56.485 | | | 62.90 40.31 | A A | 0 |
| ATOM | 179 | ŏ | | | 148 | | -56.989 | | | 39.68 | A | Ö |
| ATOM | 180 | N | | | 149 | | -55.187 | | | 37.70 | A | И |
| ATOM | 181 | CA | | | 149 | | -54.236 | | | 36.17 | A | C |
| ATOM | 182 | CB | | | 149 | | -52.976 | | | 38.73 | A | C |
| ATOM | 183 | CG | | | 149 | | -51.920 | | | 39.39 | A | c |
| ATOM | 184 | CD1 | LEU | | | | -52.465 | | | 46.05 | A | Ċ |
| ATOM | 185 | CD2 | LEU | Α | 149 | | -50.660 | | 1.00 | 40.68 | A | С |
| ATOM | 186 | С | LEU | Α | 149 | | -53.920 | | 1.00 | 35.83 | A | С |
| ATOM | 187 | 0 | LEU | Α | 149 | | -54.217 | | 1.00 | 37.60 | A | 0 |
| MOTA | 188 | N | ALA | Α | 150 | 262.029 | -53.321 | 102.228 | 1.00 | 37.02 | A | N |
| MOTA | 189 | CA | | | 150 | | -53.041 | | 1.00 | 35.35 | A | С |
| ATOM | 190 | CB | | | 150 | | -54.345 | | 1.00 | 48.80 | A | С |
| ATOM | 191 | С | | | 150 | | -52.334 | | 1.00 | 44.17 | A | С |
| MOTA | 192 | 0 | | | 150 | 261.665 | | 99.566 | | 41.00 | A | 0 |
| ATOM | 193 | N | | | 151 | 263.619 | | 99.666 | | 47.00 | A | N |
| ATOM | 194 | CA | ARG | | | 263.319 | | 98.468 | | 50.37 | A | С |
| ATOM | 195 | CB | | | 151 | 263.377 | | 98.793 | | 53.91 | A | C |
| ATOM | 196 | CG | ARG | | | 262.912 | | 97.649 | | 53.96 | A | C |
| ATOM | 197 | CD | ARG | | | 262.884 | | 98.014 | | 57.39 | A - | С |
| ATOM | 198 | NE | ARG | | | 264.145 | | 98.607 | | 58.37 | A | N |
| ATOM | 199 | CZ | | | 151 | 264.561 | | 98.572 | | 58.07 | A | C |
| ATOM | 200 | | ARG | | | 263.814 | | 97.969 | | 56.20 | A | N |
| ATOM ATOM | 201 202 | NH2 C | ARG | | | 265.718 | | 99.131 | | 55.48 | A n | N |
| VI ON | 202 | C | ARG | A | インエ | 264.311 | -2T.05T | 97.348 | 1.00 | 55.38 | A | С |
| | | | | | | | | | | | | |

| MOTA | 203 | 0 | ARG | А | 151 | 265.503 | -51.247 | 97.625 | 1 00 | 60.78 | 7 | 4 0 | • |
|------|-------|-----|-----|---|-----|---------|---------|----------------|------|-------|---|------------|---|
| | 204 | N | | | 152 | | -51.059 | | | | | | |
| ATOM | | | | | | | | | | 54.28 | | N | |
| ATOM | 205 | CA | | | 152 | | -51.366 | | 1.00 | 54.46 | 2 | 7 C | |
| MOTA | 206 | CB | GLU | Ą | 152 | 263.811 | -51.817 | 93.823 | 1.00 | 60.23 | 1 | 4 C | ; |
| ATOM | 207 | CG | GLU | A | 152 | 264.520 | -52.780 | 92.888 | 1.00 | 67.69 | 7 | A C | : |
| ATOM | 208 | CD | GLU | Δ | 152 | 265.617 | -52.120 | 92.087 | | 75.21 | | . c | |
| | 209 | OE1 | | | | | -52.020 | | | | | | |
| ATOM | | | | | | | | 92.593 | | 78.70 | | 4 0 | |
| MOTA | 210 | | GLU | | | | -51.689 | 90.951 | 1.00 | 76.28 | 7 | 4 0 | , |
| MOTA | 211 | C | GLU | Α | 152 | 265.436 | -50.117 | 94.598 | 1.00 | 54.18 | 2 | A C | ; |
| ATOM | 212 | 0 | GLU | Α | 152 | 264.868 | -49.045 | 94.388 | 1.00 | 55.50 | 7 | A 0 |) |
| ATOM | 213 | N | | | 153 | | -50.275 | | | 55.96 | | A N | |
| | | | | | | | | | | | | | |
| MOTA | 214 | CA | | | 153 | | -49.115 | | | 57.21 | | 4 C | |
| ATOM | 215 | СВ | | | 153 | | -49.471 | | 1.00 | 56.21 | 7 | A C | |
| ATOM | 216 | CG | LYS | A | 153 | 269.661 | -49.042 | 95.586 | 1.00 | 49.03 | 2 | Y C | : |
| ATOM | 217 | CD | LYS | Α | 153 | 270.821 | -49.929 | 95.975 | 1.00 | 56.59 | 7 | A C | ; |
| MOTA | 218 | CE | | | 153 | 271.022 | -49.981 | | | 62.23 | | Ā C | |
| ATOM | 219 | NZ | | | 153 | | -50.704 | | | | | | |
| | | | | | | | | | | 63.82 | | A N | |
| ATOM | 220 | C | | | 153 | | -48.233 | - - | | 60.69 | 1 | <i>Y</i> C | ; |
| MOTA | 221 | 0 | LYS | Ą | 153 | 267.418 | -47.029 | | 1.00 | 68.16 | 1 | <i>A</i> 0 |) |
| ATOM | 222 | N | GLN | Α | 154 | 266.890 | -48.704 | 91.909 | 1.00 | 60.83 | 7 | A N | I |
| ATOM | 223 | CA | GLN | А | 154 | 266.722 | -47.630 | | | 60.63 | | À C | |
| ATOM | 224 | CB | | | 154 | | -48.015 | | | | | | |
| | | | | | | | | | | 65.34 | | 4 C | |
| MOTA | 225 | CG | | | 154 | | -48.908 | | | 73.31 | 1 | A C | |
| ATOM | 226 | CD | GLN | A | 154 | 268.842 | -49.643 | 88.514 | 1.00 | 76.62 | 2 | A C | ; |
| ATOM | 227 | OE1 | GLN | Α | 154 | 268.751 | -49.059 | 87.368 | 1.00 | 77.22 | 1 | 4 0 |) |
| ATOM | 228 | NE2 | GLN | Α | 154 | | -50.963 | | | 79.75 | | A N | |
| MOTA | 229 | C | | | 154 | | -47.279 | | | 58.41 | | À C | |
| | | | | | | | | | | | | | |
| ATOM | 230 | 0 | | | 154 | | -46.135 | | | 66.80 | | 7 0 | |
| ATOM | 231 | N | | | 155 | | -48.297 | | 1.00 | 63.11 | 2 | A N | ĺ |
| ATOM | 232 | CA | SER | Α | 155 | 263.012 | -48.182 | 90.986 | 1.00 | 57.08 | 2 | A C | : |
| ATOM | 233 | CB | SER | Α | 155 | 262.438 | -49.593 | 90.891 | 1.00 | 57.59 | 2 | 4 C | • |
| ATOM | 234 | ŌG | | | 155 | | -49.532 | | | 71.09 | | 4 0 | |
| | | | | | | | | | | | | | |
| ATOM | 235 | С | | | 155 | | -47.454 | | | 54.17 | | 7 C | |
| MOTA | 236 | 0 | | | 155 | | -46.653 | | 1.00 | 41.48 | 2 | <i>Y</i> 0 |) |
| ATOM | 237 | N | LYS | A | 156 | 262.919 | -47.739 | 93.368 | 1.00 | 54.36 | 1 | A N | [|
| ATOM | 238 | CA | LYS | Α | 156 | 262,415 | -47.187 | 94.614 | 1.00 | 65.54 | 2 | 4 C | |
| ATOM | 239 | CB | | | 156 | | -45,687 | | | 68.88 | | . c | |
| ATOM | 240 | CG | | | | | -44.809 | | | | | | |
| | | | | | 156 | | | | | 68.98 | | 1 C | |
| ATOM | 241 | CD | | | 156 | | -43.342 | | | 65.67 | 2 | 7 C | |
| ATOM | 242 | CE | LYS | Α | 156 | 262.170 | -42.850 | 93.529 | 1.00 | 62.20 | 2 | Y C | : |
| ATOM | 243 | NZ | LYS | Α | 156 | 261.774 | -41.416 | 93.679 | 1.00 | 56.13 | 2 | N A | 1 |
| ATOM | 244 | С | LYS | Α | 156 | | -47.958 | | | 64.77 | | . C | |
| ATOM | 245 | ō | | | 156 | | -47.485 | | | | | | |
| | | | | | | | | | | 68.30 | 7 | | |
| ATOM | 246 | N | | | 157 | | -49.159 | | | 62.48 | 7 | 7 N | i |
| MOTA | 247 | CA | PHE | Α | 157 | 259.891 | -50.051 | 94.679 | 1.00 | 52.64 | 7 | Y C | ; |
| ATOM | 248 | CB | PHE | Α | 157 | 259.878 | -51.110 | 93.580 | 1.00 | 54.51 | 2 | 7 C | : |
| ATOM | 249 | CG | PHE | Α | 157 | 258,621 | -51.933 | 93.525 | 1.00 | 52.32 | 7 | , c | , |
| ATOM | 250 | | PHE | | | | -51.694 | | | 54.81 | Ī | | |
| ATOM | 251 | | | | 157 | | -52.950 | | | | | | |
| | | | | | | | | | | 55.89 | | 7 C | |
| ATOM | 252 | | PHE | | | | -52.451 | | | 53.63 | 7 | | |
| ATOM | 253 | CE2 | PHE | Α | 157 | 257.232 | -53.719 | 94.401 | | 54.27 | Į | 7 C | : |
| ATOM | 254 | CZ | PHE | Α | 157 | 256.286 | -53.467 | 93.419 | 1.00 | 58.00 | I | C | |
| MOTA | 255 | С | PHE | Α | 157 | 260.015 | -50.719 | 96.056 | | 51.79 | Į | | |
| ATOM | 256 | Ō | | | 157 | | -51.370 | | | 47.35 | Į | | |
| | 257 | | | | | | | | | | | | |
| MOTA | | N | | | 158 | | -50.539 | | | 50.33 | Į | | |
| MOTA | 258 | CA | ILE | Α | 158 | | -51.137 | | 1.00 | 48.14 | I | , C | : |
| ATOM | 259 | CB | ILE | Α | 158 | 258.329 | -50.196 | 99.284 | 1.00 | 48.26 | I | , C | |
| ATOM | 260 | CG2 | ILE | Α | 158 | 257.863 | -50.988 | 100.478 | 1.00 | 42.57 | I | | |
| ATOM | 261 | | ILE | | | | -49.205 | | | 48.74 | Į | | |
| | | | | | | | | | | | | | |
| ATOM | 262 | | ILE | | | | | 100.849 | | 60.25 | P | | |
| MOTA | 263 | С | | | 158 | | -52.530 | | | 52.33 | F | , C | |
| MOTA | 264 | 0 | ILE | Α | 158 | | -52.732 | 97.635 | 1.00 | 50.55 | 7 | . 0 | , |
| ATOM | 265 | N | LEU | A | 159 | 259.034 | -53.472 | 98.823 | | 52.37 | P | | |
| MOTA | 266 | CA | | | 159 | | -54.858 | 98.835 | | 48.01 | P | | |
| ATOM | 267 | СВ | | | 159 | | -55.530 | 97.663 | | | | | |
| | | | | | | | | | | 49.17 | P | | |
| MOTA | 268 | CG | | | 159 | | -55.019 | 97.480 | | 47.74 | P | | |
| ATOM | 269 | | LEU | | | | -55.880 | 98.307 | 1.00 | 46.92 | P | . с | |
| ATOM | 270 | CD2 | LEU | Α | 159 | 261.150 | -55.055 | 96.008 | 1.00 | 47.94 | P | . с | |
| ATOM | 271 | С | | | 159 | | | 100.111 | | 44.03 | P | | |
| ATOM | 272 | ŏ | | | 159 | | | 100.931 | | 48.23 | A | | |
| | _ , _ | ~ | 0 | | | | | 100.331 | 1.00 | 30.43 | | . 0 | |

| ATOM | 273 | N | ALA | Α | 160 | 258.889 | -56.765 | 100.280 | 1.00 | 43.85 | Α | N |
|--------------|------------|---------|-----|---|------------|---------|--------------------|---------|------|----------------|--------|---|
| ATOM | 274 | CA | ALA | Α | 160 | 259.347 | -57.465 | 101.474 | 1.00 | 37.28 | A | С |
| ATOM | 275 | CB | ALA | Α | 160 | 258.187 | -58.117 | 102.184 | 1.00 | 41.03 | A | С |
| MOTA | 276 | С | ALA | A | 160 | 260.346 | -58.531 | 101.030 | 1.00 | 43.40 | A | С |
| ATOM | 277 | 0 | ALA | A | 160 | 260.084 | -59.301 | 100.096 | 1.00 | 40.92 | Α | 0 |
| ATOM | 278 | N | LEU | Α | 161 | 261.494 | -58.566 | 101.693 | 1.00 | 46.08 | Α | N |
| ATOM | 279 | CA | LEU | Α | 161 | 262.564 | -59.520 | 101.378 | 1.00 | 44.64 | A | С |
| MOTA | 280. | CB | LEU | Α | 161 | 263.916 | -58.794 | 101.334 | 1.00 | 47.23 | A | С |
| ATOM | 281 | CG | LEU | Α | 161 | 264.865 | -59.050 | 100.188 | 1.00 | 47.49 | Α | C |
| ATOM | 282 | CD1 | LEU | A | 161 | 264.153 | -58.846 | 98.870 | 1.00 | 42.04 | Α | С |
| ATOM | 283 | CD2 | LEU | Α | 161 | 266.031 | -58.125 | 100.309 | 1.00 | 46.85 | A | С |
| MOTA | 284 | С | LEU | Α | 161 | 262.607 | -60.592 | 102.441 | 1.00 | 45.60 | A | C |
| ATOM | 285 | 0 | LEU | A | 161 | 263.013 | -60.338 | 103.570 | 1.00 | 56.35 | A | 0 |
| ATOM | 286 | N | LYS | Α | 162 | 262.194 | -61.801 | 102.078 | 1.00 | 46.81 | A | N |
| ATOM | 287 | CA | LYS | A | 162 | 262.178 | -62.940 | 103.009 | 1.00 | 41.78 | Α | С |
| MOTA | 288 | CB | LYS | Α | 162 | 261.104 | -63.922 | 102.585 | 1.00 | 37.22 | A | С |
| ATOM | 289 | CG | LYS | Α | 162 | 260.826 | -65.007 | 103.588 | 1.00 | 34.96 | A | C |
| ATOM | 290 | CD | LYS | Α | 162 | 259.600 | ~65.804 | 103.219 | 1.00 | 30.75 | Α | C |
| ATOM | 291 | CE | LYS | A | 162 | 259.522 | -67.056 | 104.081 | 1.00 | 32.45 | A | С |
| MOTA | 292 | NZ | LYS | Α | 162 | 258.194 | -67.801 | 103.796 | 1.00 | 32.97 | A | N |
| MOTA | 293 | С | LYS | Α | 162 | 263.521 | -63.634 | 103.018 | 1.00 | 43.17 | Α | C |
| ATOM | 294 | 0 | LYS | Ą | 162 | 263.869 | -64.350 | 102.087 | 1.00 | 50.65 | A | 0 |
| MOTA | 295 | N | VAL | Α | 163 | 264.299 | -63.369 | 104.049 | 1.00 | 47.41 | А | N |
| ATOM | 296 | CA | VAL | A | 163 | 265.625 | -63.965 | 104.187 | 1.00 | 50.56 | Α | C |
| ATOM | 297 | CB | VAL | Α | 163 | 266.539 | -63.091 | 105.120 | 1.00 | 49.49 | A | C |
| ATOM | 298 | CG1 | VAL | A | 163 | 267.951 | -63.664 | 105.180 | 1.00 | 43.15 | А | С |
| MOTA | 299 | CG2 | VAL | A | 163 | 266.555 | -61.660 | 104.586 | 1.00 | 46.95 | A | С |
| MOTA | 300 | С | VAL | A | 163 | 265.570 | -65.371 | 104.756 | 1.00 | 48.41 | A | C |
| ATOM | 301 | 0 | VAL | A | 163 | | -65.586 | | 1.00 | 53.08 | A | 0 |
| MOTA | 302 | N | LEU | A | 164 | 266.195 | -66.329 | 104.085 | 1.00 | 53.99 | A | N |
| MOTA | 303 | CA | LEU | A | 164 | 266.261 | -67.732 | 104.569 | 1.00 | 55.36 | A | С |
| ATOM | 304 | CB | LEU | A | 164 | 265.516 | -68.657 | 103.598 | 1.00 | 54.99 | A | С |
| MOTA | 305 | CG | | | 164 | | -68.154 | | 1.00 | 57.06 | A | |
| MOTA | 306 | | LEU | | | | | 101.535 | 1.00 | 57.49 | A | |
| ATOM | 307 | | LEU | | | | -68.851 | | | 55.47 | A | |
| ATOM | 308 | С | | | .164 | | -68.188 | | 1.00 | 52.23 | A | C |
| ATOM | 309 | 0 | | | 164 | | | 103.745 | | 50.98 | A | 0 |
| MOTA | 310 | N | | | 165 | | -68.800 | | | 52.15 | A | |
| ATOM | 311 | CA | | | 165 | | | 105.892 | | 51.87 | A | C |
| ATOM | 312 | CB | | | 165 | | -69.322 | | | 54.79 | A | |
| ATOM | 313 | CG | | | 165 | | | 107.875 | | 59.43 | A | |
| MOTA | 314 | | PHE | | | | | 108.426 | | 61.03 | A | |
| MOTA | 315 | | PHE | | | | | 107.769 | | 59.15 | A | |
| MOTA | 316 | | PHE | | | | | 108.856 | | 59.31 | A | |
| MOTA | 317 | | PHE | | | | | 108.196 | | 59.42 | A | C |
| ATOM | 318 | CZ | | | 165 | | -65.412 | | | 60.41 | A | C |
| ATOM | 319 320 | C | | | 165 165 | | -70.683 -71.654 | 105.267 | | 52.40 45.64 | A | |
| ATOM ATOM | 321 | 0 | | | 166 | | | 103.673 | | 52.32 | A | |
| ATOM | 322 | N CA | | | 166 | | | 104.520 | | 53.94 | A A | |
| ATOM | 323 | CB | | | 166 | | | 102.708 | | 47.98 | A | |
| ATOM | 324 | CG | | | 166 | | | 101.498 | | 41.92 | A | |
| MOTA | 325 | CD | | | 166 | | | 100.383 | | 38.85 | A A | |
| MOTA | 326 | CE | | | 166 | | -70.201 | 99.345 | | 31.90 | A | |
| ATOM | 327 | NZ | | | 166 | 273.477 | | 98.252 | | 43.47 | Ā | |
| ATOM | 328 | C | | | 166 | | | 104.740 | | 51.94 | A | |
| ATOM | 329 | ŏ | | | 166 | | | 104.743 | | 62.20 | A | |
| ATOM | 330 | N | | | 167 | | | 105.659 | | 51.64 | A | |
| ATOM | 331 | CA | | | 167 | | | 106.682 | | 51.81 | A | C |
| MOTA | 332 | CB | | | 167 | | | 107.670 | | 53.31 | A | č |
| ATOM | 333 | C | | | 167 | | | 107.369 | | 53.85 | A | Ċ |
| ATOM | 334 | ō | | | 167 | 271.105 | | | | 57.18 | A | 0 |
| ATOM | 335 | N | | | 168 | 270.318 | | | | 59.28 | A | N |
| MOTA | 336 | CA | | | 168 | 269.139 | | | | 59.95 | A | C |
| ATOM | 337 | CB | | | 168 | 268.348 | | | | 66.12 | A | C |
| ATOM | 338 | CG | | | 168 | 268.398 | | | | 72.61 | A | Ċ |
| ATOM | 339 | CD | | | 168 | 267.038 | | | | 77.64 | A | č |
| MOTA | 340 | | GLN | | | 266.542 | | | | 76.82 | A | Ö |
| ATOM | 341 | | GLN | | | 266.432 | | | | 72.17 | A | Ŋ |
| ATOM | 342 | С | | | 168 | 268.221 | | | | 55.73 | A | C |
| | | | | | | | | | | | | |

| ATOM | 343 | 0 | GLN | | | 267.646 | -75.736 | 108.043 | 1.00 53.22 | A | 0 |
|--------------|------------|----------|------------|---|-----|-----------------|--------------------|------------------|--------------------------|--------|--------|
| ATOM | 344 | N | LEU | | | | -74.262 | | 1.00 47.44 | A | N |
| MOTA | 345 | CA | LEU | | | | -74.954 | | 1.00 53.18 | A | С |
| ATOM ATOM | 346 347 | CB CG | LEU | | | | -74.247 -72.939 | | 1.00 46.05 | A | C |
| ATOM | 348 | | LEU | | | 266.858 | -72.939 -72.184 | 104.055 | 1.00 47.35 1.00 45.64 | A A | C |
| ATOM | 349 | | LEU | | | | -73.224 | | 1.00 44.94 | A | c |
| MOTA | 350 | С | LEU | A | 169 | | -76.381 | | 1.00 53.79 | A | Ċ |
| ATOM | 351 | 0 | LEU | | | | -77.361 | | 1.00 54.87 | A | 0 |
| ATOM | 352 | N | GLU | | | | -76.488 | | 1.00 54.40 | A | N |
| ATOM ATOM | 353 354 | CA CB | GLU GLU | | | | -77.771 | | 1.00 58.30 | A | C |
| ATOM | 355 | CG | GLU | | | | -77.587 -77.158 | | 1.00 57.36 1.00 66.04 | A A | C |
| ATOM | 356 | CD | | | 170 | | -76.836 | | 1.00 73.19 | A | Č |
| MOTA | 357 | | GLU | | | | -77.755 | | 1.00 76.86 | A | ō |
| ATOM | 358 | | GLU | | | | -75.670 | | 1.00 77.40 | A | 0 |
| ATOM | 359 | C | | | 170 | | -78.643 | | 1.00 60.58 | A | С |
| ATOM ATOM | 360 361 | И | LYS | | 170 | | -79.730 -78.162 | | 1.00 71.27 | A | 0 |
| ATOM | 362 | CA | LYS | | | | -78.942 | | 1.00 59.38 1.00 59.74 | A A | N C |
| ATOM | 363 | CB | LYS | | | | -78.118 | | 1.00 58.50 | Ā | c |
| ATOM | 364 | C | LYS | A | 171 | 268.409 | -79.500 | 108.655 | 1.00 62.87 | A | č |
| MOTA | 365 | 0 | LYS | | | | -80.438 | | 1.00 65.46 | A | 0 |
| ATOM | 366 | N | ALA | | | | -78.939 | | 1.00 58.04 | A | N |
| ATOM ATOM | 367 368 | CA CB | ALA ALA | | | | -79.373 -78.157 | | 1.00 55.58 1.00 44.25 | A | C |
| ATOM | 369 | C | ALA | | | | -80.129 | | 1.00 44.25 | A A | C |
| ATOM | 370 | 0 | ALA | A | 172 | 264.406 | -80.699 | 107.038 | 1.00 63.97 | A | ő |
| ATOM | 371 | N | | | 173 | | -80.108 | | 1.00 59.05 | A | N |
| ATOM | 372 | CA | | | 173 | | -80.806 | | 1.00 58.57 | A | С |
| ATOM ATOM | 373 374 | С 0 | GLY | | | | -80.290 -81.045 | 104.096 | | A | C |
| ATOM | 375 | Ŋ | VAL | | | | -78.983 | | 1.00 57.22 1.00 52.27 | A A | О И |
| ATOM | 376 | CA | VAL | | | | -78.389 | | 1.00 52.27 | A | C |
| ATOM | 377 | CB | VAL | | | | -77.420 | | 1.00 44.57 | A | Ċ |
| ATOM | 378 | | VAL | | | | -78.172 | | 1.00 45.83 | A | С |
| ATOM ATOM | 379 380 | CGZ | VAL VAL | | | | -76.374 -77.628 | | 1.00 43.22 | A | C |
| ATOM | 381 | ŏ | VAL | | | | -76.679 | | 1.00 55.27 1.00 62.81 | A A | C |
| ATOM | 382 | N | GLU | | | 264.577 | -78.044 | 101.548 | 1.00 50.98 | A | N |
| MOTA | 383 | CA | GLU | | | | -77.393 | 100.296 | 1.00 52.00 | A | С |
| ATOM | 384 | CB CG | GLU | | | | -77.994 | 99.721 | 1.00 47.79 | A | C |
| ATOM ATOM | 385 386 | CD | GLU GLU | | | | -77.861 -79.101 | | 1.00 59.64 1.00 59.83 | A | C |
| ATOM | 387 | | GLU | | | | -79.948 | | 1.00 59.83 | A A | 0 |
| ATOM | 388 | | GLU | A | 175 | | -79.219 | | 1.00 70.43 | A | ŏ |
| ATOM | 389 | С | GLU | | | | -77.526 | 99.266 | 1.00 51.17 | A | С |
| ATOM | 390 | 0 | GLU | | | | -76.642 | 98.463 | 1.00 57.75 | A | 0 |
| ATOM ATOM | 391 392 | N CA | HIS HIS | | | | -78.661 -78.920 | 99.266 98.312 | 1.00 60.20 1.00 61.34 | A | N |
| ATOM | 393 | CB | HIS | | | | -80.414 | 98.276 | 1.00 62.47 | A A | C |
| MOTA | 394 | CG | HIS | | | | -80.959 | 99.579 | 1.00 70.92 | A | č |
| MOTA | 395 | | HIS | | | | -81.020 | | 1.00 68.70 | A | С |
| ATOM | 396 | | HIS | | | 260.020 | | 99.740 | 1.00 72.07 | A | N |
| ATOM ATOM | 397 398 | | HIS HIS | | | | -81.925 -81.625 | | 1.00 75.43 | A | C |
| ATOM | 399 | C | HIS | | | 260.828 | | 98.620 | 1.00 77.22 1.00 60.76 | A A | И С |
| ATOM | 400 | 0 | HIS | | | 260.058 | | 97.733 | 1.00 64.86 | A | ō |
| ATOM | 401 | N | GLN | | | 260.607 | | 99.886 | 1.00 63.60 | A | N |
| ATOM | 402 | CA | GLN | | | | -76.993 | | 1.00 59.32 | A | C |
| ATOM ATOM | 403 404 | CB CG | GLN GLN | | | 258 577 | -77.080 -78.484 | 102.756 | 1.00 65.79 | A | C |
| ATOM | 405 | CD | GLN | | | | -78.896 | | 1.00 78.25 1.00 84.93 | A A | C |
| ATOM | 406 | | GLN | | | | -79.822 | | 1.00 89.62 | A | 0 |
| ATOM | 407 | NE2 | GLN | A | 177 | 259.316 | -78.274 | | 1.00 87.76 | A | N |
| ATOM | 408 | C | GLN | | | 259.647 | | 99.730 | 1.00 54.25 | Α | С |
| ATOM ATOM | 409 410 | M O | GLN LEU | | | 258.739 | | 99.073 | 1.00 51.39 | A | 0 |
| ATOM | 411 | n Ca | LEU | | | 260.844 261.123 | | 99.942 99.474 | 1.00 45.84 1.00 49.49 | A A | N C |
| ATOM | 412 | CB | LEU | | | 262.514 | | 99.900 | 1.00 49.49 | A | C |
| | | | | | | | - | | - | | - |

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| ATOM | 413 | CG | LEU | A | 178 | 263.032 | -71.858 | 99.325 | 1.00 | 49.26 | A | С |
|--------------|------------|----------|-----|---|-----|---------|--------------------|------------------|------|----------------|--------|--------|
| ATOM | 414 | CD1 | LEU | | | | -70.693 | 99.584 | | 37.20 | A | c |
| ATOM | 415 | CD2 | LEU | Α | 178 | | -71.557 | 99.950 | | 46.43 | A | C |
| MOTA | 416 | С | LEU | Α | 178 | | -73.631 | 97.939 | | 46.87 | A | C |
| ATOM | 417 | 0 | LEU | A | 178 | | -72.659 | 97.280 | 1.00 | 52.87 | A | 0 |
| ATOM | 418 | N | ARG | Α | 179 | 261.314 | -74.778 | 97.360 | 1.00 | 52.38 | A | N |
| ATOM | 419 | CA | ARG | A | 179 | 261.258 | -74.887 | 95.908 | 1.00 | 48.78 | A. | С |
| ATOM | 420 | CB | ARG | A | 179 | 261.877 | -76.207 | 95.443 | 1.00 | 55.74 | A | С |
| ATOM | 421 | CG | ARG | | | 262.661 | -76.085 | 94.149 | 1.00 | 55.19 | A | С |
| ATOM | 422 | CD | ARG | Α | 179 | 263.898 | -77.002 | 94.178 | 1.00 | 71.41 | A | C |
| ATOM | 423 | NE | ARG | Α | 179 | 264.829 | -76.685 | 93.086 | 1.00 | 73.48 | A | N |
| ATOM | 424 | CZ | ARG | Α | 179 | 264.827 | -77.258 | 91.873 | 1.00 | 77.16 | A | С |
| ATOM | 425 | | ARG | | | 263.941 | -78.208 | 91.565 | 1.00 | 70.26 | A | N |
| MOTA | 426 | | ARG | | | 265.709 | -76.874 | 90.951 | 1.00 | 75.62 | A | N |
| MOTA | 427 | С | | | 179 | | -74.758 | 95.383 | | 46.80 | A | С |
| ATOM | 428 | 0 | | | 179 | | -74.009 | 94.443 | | 37.96 | A | 0 |
| ATOM | 429 | N | ARG | | | | -75.494 | 95.988 | | 41.56 | A | N |
| ATOM | 430 | CA | ARG | | | | -75.451 | 95.630 | | 46.45 | A | С |
| MOTA | 431 | CB | | | 180 | | -76.543 | 96.386 | | 47.01 | A | C |
| ATOM | 432 | CG | | | 180 | | -77.762 | 95.546 | | 51.52 | A | C |
| ATOM | 433 | CD | | | 180 | | -78.783 | 96.257 | | 53.97 | A | С |
| ATOM ATOM | 434 | NE | | | 180 | | -79.863 | 96.824 | | 69.57 | A. | N |
| | 435 436 | CZ | ARG | | 180 | | -79.849 -78.796 | 98.046 | | 76.20 | A | C |
| ATOM ATOM | 437 | | ARG | | | | -80.893 | 98.846 | | 85.82 | A | N |
| MOTA | 438 | C | | | 180 | | -74.100 | 98.475 95.969 | | 82.98 48.19 | A | N |
| ATOM | 439 | Ö | | | 180 | | -73.556 | 95.189 | | 55.26 | A A | С 0 |
| ATOM | 440 | N | | | 181 | | -73.560 | 97.130 | | 49.77 | A | Ŋ |
| ATOM | 441 | CA | | | 181 | | -72.279 | 97.536 | | 48.24 | A | C |
| MOTA | 442 | CB | GLU | | | | -71.820 | 98.841 | | 51.28 | A | C |
| ATOM | 443 | CG | | | 181 | | -70.425 | 99.303 | | 55.39 | A | C |
| ATOM | 444 | CD | GLU | | | | -70.042 | | | 57.20 | A | Č |
| ATOM | 445 | OE1 | GLU | | | | -70.904 | | | 46.80 | A | ō |
| MOTA | 446 | OE2 | GLU | Α | 181 | | -68.871 | | | 56.40 | A | ō |
| ATOM | 447 | C | GLU | Α | 181 | | -71.259 | 96.430 | | 49.63 | A | С |
| MOTA | 448 | 0 | GLU | A | 181 | 256.044 | -70.571 | 95.930 | 1.00 | 44.79 | A | 0 |
| ATOM | 449 | N | VAL | Α | 182 | 258.227 | -71.191 | 96.037 | 1.00 | 46.11 | A | N |
| ATOM | 450 | CA | VAL | Α | 182 | 258.659 | -70.228 | 95.035 | 1.00 | 45.55 | A | С |
| ATOM | 451 | CB | | | 182 | | -70.266 | 94.833 | 1.00 | 40.91 | A | С |
| ATOM | 452 | | VAL | | | | -69.403 | 93.678 | | 38.12 | A | С |
| MOTA | 453 | | VAL | | | | -69.730 | 96.059 | | 51.08 | A | С |
| ATOM | 454 | C | VAL | | | | -70.443 | 93.695 | | 46.82 | A | С |
| ATOM | 455 | 0 | VAL | | | | -69.483 | 93.056 | | 40.29 | A | 0 |
| ATOM | 456 | N | | | 183 | | -71.690 | 93.237 | | 48.08 | A | N |
| MOTA | 457 | CA | | | 183 | | -72.012 | 91.968 | | 52.62 | A | C |
| ATOM ATOM | 458 459 | CB CG | GLU | | 183 | | -73.478 | 91.608 | | 56.60 | A | С |
| ATOM | 460 | CD | GLU | | | | -73.784 -75.283 | 90.808 90.746 | | 70.69 | A | C |
| ATOM | 461 | | GLU | | | | -76.011 | 90.397 | | 77.34 83.76 | A | C |
| ATOM | 462 | | GLU | | | | -75.727 | 91.052 | | 82.45 | A A | 0 |
| ATOM | 463 | C | GLU | | | | -71.754 | 91.912 | | 49.85 | Ā | C |
| MOTA | 464 | Ō | GLU | | | | -71.138 | 90.947 | | 46.36 | A | ō |
| MOTA | 465 | N | ILE | | | | -72.317 | 92.898 | | 46.74 | A | N |
| ATOM | 466 | CA | ILE | | | | -72.157 | 92.965 | | 43.86 | A | Ċ |
| ATOM | 467 | CB | ILE | Α | 184 | | -72.962 | 94.115 | | 40.26 | A | c |
| MOTA | 468 | CG2 | ILE | | | | -72.714 | 94.209 | | 29.84 | A | c |
| ATOM | 469 | CG1 | ILE | Α | 184 | 253.313 | -74.446 | 93.860 | | 36.80 | A | С |
| ATOM | 470 | CD1 | ILE | Α | 184 | 252.748 | -75.369 | 94.961 | | 40.80 | A | С |
| MOTA | 471 | С | ILE | Α | 184 | 253.221 | -70.713 | 93.099 | 1.00 | 46.29 | A | С |
| ATOM | 472 | 0 | ILE | | | 252.448 | -70.199 | 92.284 | 1.00 | 49.47 | A | 0 |
| ATOM | 473 | N | GLN | | | | -70.054 | 94.132 | | 49.28 | A | N |
| ATOM | 474 | CA | GLN | | | | -68.666 | 94.388 | | 52.47 | Ą | С |
| ATOM | 475 | СВ | GLN | | | | -68.189 | 95.721 | | 44.73 | A. | С |
| ATOM | 476 | CG | GLN | | | | -67.168 | 96.526 | | 48.30 | A | С |
| ATOM | 477 | CD | GLN | | | | -66.745 | 97.745 | | 54.47 | A | С |
| ATOM | 478 | | GLN | | | | ~67.516 | 98.331 | | 61.67 | A | 0 |
| MOTA | 479 | | GLN | | | | -65.501 | 98.201 | | 56.50 | A | N |
| ATOM | 480 | C | GLN | | | | -67.716 | 93.231 | | 50.63 | A | C |
| ATOM | 481 | 0 | GLN | | | | -66.780 | 92.894 | | 52.61 | A | 0 |
| ATOM | 482 | N | SER | A | тяр | ∠54.843 | -67.972 | 92.610 | T.00 | 47.27 | A | N |

| ATOM | 483 | CA | SER | A | 186 | 255.315 | -67.114 | 91.541 | 1.00 | 52.03 | ; | A | С |
|--------------|------------|----------|------------|---|------------|---------|--------------------|------------------|------|----------------|---|---------|--------|
| MOTA | 484 | CB | SER | Α | 186 | 256.692 | -67.586 | 91.048 | 1.00 | 51.09 | | A | С |
| MOTA | 485 | OG | SER | Α | 186 | 256.609 | -68.877 | 90.496 | 1.00 | 54.11 | i | A | 0 |
| MOTA | 486 | С | | | 186 | | -67.050 | 90.373 | | 51.30 | | A | С |
| ATOM | 487 | 0 | SER | | | 254.116 | | 89.812 | | 53.71 | | A | 0 |
| ATOM | 488 | N | HIS | | | 253.774 | | 90.001 | | 55.86 | | A | N |
| ATOM | 489 | CA | HIS | | | | -68.233 | 88.883 | | 57.28 | | A | C |
| MOTA | 490 | CB | HIS | | | | -69.605 | 88.190 | | 68.44 | | A. | C |
| ATOM | 491 | CG | HIS | | | | -69.866 | 87.541 | | 77.26 | | A | C |
| MOTA | 492 | | HIS HIS | | | 255.147 | -71.114 | 86.892 87.532 | | 78.77 80.45 | | A | C |
| ATOM ATOM | 493 494 | | HIS | | | | -71.114 | 86.911 | | 81.91 | | A A | N C |
| ATOM | 495 | | HIS | | | | -69.802 | 86.512 | | 81.51 | | A A | N |
| ATOM | 496 | C | | | 187 | | -67.953 | 89.300 | | 57.51 | | A | C |
| MOTA | 497 | ō | _ | | 187 | | -68.154 | 88.529 | | 60.26 | | A | ŏ |
| ATOM | 498 | N | | | 188 | | -67.497 | 90.530 | | 59.97 | | A | N |
| ATOM | 499 | CA | | | 188 | | -67.189 | 91.028 | | 56.67 | | A | С |
| ATOM | 500 | CB | LEU | A | 188 | 249.832 | -67.488 | 92.511 | 1.00 | 57.07 | | A | С |
| MOTA | 501 | CG | LEU | A | 188. | 248.970 | -68.663 | 92.952 | | 55.73 | | A | С |
| ATOM | 502 | | LEU | | | | -69.896 | 92.257 | | 62.61 | | Ą | С |
| ATOM | 503 | | LEU | | | | -68.827 | 94.465 | | 53.98 | | A | С |
| ATOM | 504 | С | | | 188 | | -65.728 | 90.777 | | 57.85 | | A | С |
| MOTA | 505 | 0 | | | 188 | | -64.881 | 90.799 | | 64.49 | | A - | 0 |
| ATOM | 506 | N | | | 189 | | -65.440 | 90.507 | | 59.25 | | A | N |
| ATOM | 507 508 | CA CB | | | 189 189 | | -64.067 -63.796 | 90.239 88.734 | | 63.66 64.78 | | A. | C |
| ATOM ATOM | 509 | CG | | | 189 | | -63.660 | 88.125 | | 70.33 | | A A | C |
| ATOM | 510 | CD | | | 189 | | -62.285 | 88.356 | | 70.33 | | A. | c |
| ATOM | 511 | NE | | | 189 | | -61.937 | 87.301 | | 81.14 | | A. | N |
| MOTA | 512 | CZ | | | 189 | | -60.923 | 86.432 | | 82.52 | | A. | C |
| ATOM | 513 | NH1 | ARG | A | 189 | 249.636 | -60.138 | 86.478 | | 79.99 | | A | N |
| ATOM | 514 | NH2 | ARG | Α | 189 | 251.658 | -60.669 | 85.521 | 1.00 | 82.64 | | A | N |
| MOTA | 515 | С | ARG | Α | 189 | 246.469 | -63.844 | 90.761 | 1.00 | 59.43 | | A | C |
| MOTA | 516 | 0 | | | 189 | | -64.167 | 90.072 | | 61.20 | | A | 0 |
| ATOM | 517 | N | | | 190 | | -63.283 | 91.964 | | 56.49 | | A | N |
| ATOM | 518 | CA | | | 190 | | -63.075 | 92.565 | | 48.34 | | A. - | С |
| ATOM | 519 | CB | | | 190 | | -64.377 | 93.201 | | 52.70 | | A. | C |
| ATOM ATOM | 520 521 | CG | HIS | | 190 | | -64.372 -65.207 | 93.489 93.107 | | 49.06 52.53 | | A A | C |
| ATOM | 522 | | HIS | | | | -63.432 | 94.302 | | 51.06 | | A A | N |
| ATOM | 523 | | HIS | | | | -63.686 | 94.414 | | 46.17 | | A | C |
| ATOM | 524 | | HIS | | | | -64.757 | 93.697 | | 43.53 | | A | N |
| ATOM | 525 | С | HIS | Α | 190 | 245.116 | -61,998 | 93.611 | | 47.54 | | A | C |
| ATOM | 526 | 0 | HIS | A | 190 | 246.077 | -61.946 | 94.377 | 1.00 | 44.41 | | A | 0 |
| MOTA | 527 | N | | | 191 | 244.119 | -61.102 | 93.645 | 1.00 | 49.93 | | A | N |
| ATOM | 528 | CD | PRO | Α | 191 | | -61.054 | 92.749 | 1.00 | 46.91 | | A | С |
| ATOM | 529 | CA | | | 191 | | -59.992 | 94.607 | | 49.33 | | A | С |
| ATOM | 530 | CB | | | 191 | | -59.384 | 94.346 | | 50.21 | | A. | C |
| ATOM | 531 532 | CG C | | | 191 191 | | -59.644 -60.419 | 92.887 96.072 | | 48.82 | | A. | C |
| ATOM ATOM | 533 | Ö | | | 191 | | -59.719 | 96.848 | | 46.55 42.94 | | A A | C |
| ATOM | 534 | N | | | 192 | | -61.555 | 96.434 | | 42.75 | | A. | И |
| ATOM | 535 | CA | | | 192 | | -62.060 | 97.791 | | 48.46 | | A | Ĉ |
| ATOM | 536 | CB | | | 192 | | -62.678 | 98.192 | | 45.61 | | A | Ċ |
| ATOM | 537 | CG | | | 192 | 241.206 | -61.781 | 97.847 | 1.00 | 48.26 | | A | С |
| MOTA | 538 | OD1 | ASN | Α | 192 | | -61.767 | 96.724 | 1.00 | 55.77 | | A | 0 |
| ATOM | 539 | ND2 | ASN | | | | -61.020 | 98.804 | 1.00 | 48.89 | 1 | A | N |
| ATOM | 540 | С | | | 192 | | -63.085 | 97.953 | | 44.35 | | A | С |
| ATOM | 541 | 0 | | | 192 | | -64.017 | 98.747 | | 54.33 | | Α. | 0 |
| MOTA | 542 | N | | | 193 | | -62.901 | 97.204 | | 42.87 | | A. | N |
| ATOM ATOM | 543 544 | CA CB | | | 193 193 | | -63.781 -64.847 | 97.277 96.138 | | 40.40 | | A n | C |
| ATOM | 545 | | ILE | | | | -65.733 | 96.243 | | 22.41 | | A A | C |
| ATOM | 546 | | ILE | | | | -65.732 | 96.274 | | 36.30 | | A. | C |
| ATOM | 547 | | ILE | | | | -66.793 | 95.246 | | 46.23 | | A. | c |
| ATOM | 548 | C | | | 193 | | -62.944 | 97.180 | | 43.53 | | Ā | č |
| MOTA | 549 | 0 | | | 193 | | -62.176 | 96.228 | | 41.20 | | Ą | ō |
| ATOM | 550 | N | | | 194 | | -63.070 | 98.171 | 1.00 | 46.32 | 2 | Ą | N |
| MOTA | 551 | CA | | | 194 | 250.449 | | 98.168 | | 48.93 | 1 | A | С |
| ATOM | 552 | CB | LEU | A | 194 | 251.233 | -62.511 | 99.477 | 1.00 | 44.51 | 1 | A . | С |

| ATOM | 553 | CG | LEU | A | 194 | 252.485 | -61.630 | 99.579 | 1.00 | 41.08 | A | С |
|-------|-----|------|------|----|-----|---------|----------|---------|------|-------|---|-----|
| ATOM | 554 | CD1 | LEU | Α | 194 | 252,055 | -60.195 | 99.956 | 1.00 | 43.64 | A | С |
| ATOM | 555 | | LEU | | | | -62.183 | 100.655 | 1.00 | 41.05 | Α | |
| ATOM | 556 | C | LEU | | | | -62.773 | 96.988 | | 49.00 | A | |
| ATOM | 557 | 0 | LEU | | | | -63.975 | 96.826 | | 53.77 | A | |
| | 558 | N | ARG | | | | -61.823 | 96.162 | | 43.08 | A | |
| ATOM | | | | | | | | | | | | |
| ATOM | 559 | CA | ARG | | | | -62.166 | 95.023 | | 45.19 | A | |
| MOTA | 560 | CB | ARG | | | | -61.043 | 93.969 | | 43.15 | A | |
| ATOM | 561 | CG | ARG | | | | -60.913 | 93.213 | | 46.56 | A | |
| ATOM | 562 | CD | ARG | A | 195 | 251.400 | -60.798 | 91.730 | 1.00 | 59.57 | A | C |
| ATOM | 563 | NE | ARG | Α | 195 | 252.816 | -60.787 | 91.377 | 1.00 | 72.51 | Α | N |
| MOTA | 564 | CZ | ARG | A | 195 | 253.288 | -60.716 | 90.133 | 1.00 | 78.66 | A | C |
| ATOM | 565 | NH1 | ARG | Α | 195 | 252,446 | -60.646 | 89.119 | 1.00 | 80.03 | A | N |
| ATOM | 566 | | ARG | | | | -60.723 | 89.898 | | 82.29 | A | |
| ATOM | 567 | С | ARG | | | | -62.450 | 95.390 | | 44.60 | A | |
| ATOM | 568 | ō | | | 195 | | -62.001 | 96.429 | | 47.11 | A | |
| | 569 | N | | | | | -63.177 | 94.522 | | | | |
| ATOM | | | | | 196 | | | | | 48.18 | A | |
| ATOM | 570 | CA | | | 196 | | -63.465 | 94.735 | | 48.30 | A | |
| ATOM | 571 | CB | | | 196 | | -64.954 | 95.048 | | 50.39 | A | |
| ATOM | 572 | CG | | | 196 | | -65.343 | 95.383 | | 41.45 | A | |
| ATOM | 573 | | LEU | | | 258.090 | -64.804 | 96.698 | | 58.09 | A | . C |
| MOTA | 574 | CD2 | LEU | A | 196 | 257.886 | -66.788 | 95.411 | 1.00 | 44.21 | A | C |
| MOTA | 575 | С | LEU | Α | 196 | 256.799 | -63.091 | 93.432 | 1.00 | 50.04 | A | . С |
| ATOM | 576 | 0 | LEU | A | 196 | 256.887 | -63.926 | 92.532 | 1.00 | 56.48 | A | . 0 |
| ATOM | 577 | N | TYR | Α | 197 | 257.301 | -61.854 | 93.359 | | 52.17 | A | . N |
| ATOM | 578 | CA | | | 197 | | -61.330 | 92.172 | | 49.64 | A | |
| MOTA | 579 | CB | | | 197 | | -59.908 | 92.460 | | 44.72 | A | |
| ATOM | 580 | CG | | | 197 | | -59.034 | 92.959 | | 43.03 | A | |
| | 581 | CD1 | | | 197 | | -58.246 | 94.117 | | 44.46 | A | |
| ATOM | | | | | 197 | | | | | | | |
| ATOM | 582 | CE1 | | | | | -57.433 | 94.583 | | 51.15 | A | |
| ATOM | 583 | CD2 | | | 197 | | -58.978 | 92.278 | | 41.30 | A | |
| ATOM | 584 | CE2 | | | 197 | | -58.161 | 92.730 | | 50.46 | A | |
| ATOM | 585 | CZ | | | 197 | | -57.390 | 93.887 | | 52.65 | A | |
| MOTA | 586 | ОН | TYR | A | 197 | 254.234 | -56.573 | 94.338 | 1.00 | 63.16 | A | . 0 |
| ATOM | 587 | С | TYR | A | 197 | 259.142 | -62.186 | 91.684 | 1.00 | 51.16 | A | . с |
| MOTA | 588 | 0 | TYR | Α | 197 | 259.129 | -62.683 | 90.572 | 1.00 | 58.21 | A | . 0 |
| MOTA | 589 | N | GLY | A | 198 | 260.141 | -62.378 | 92.529 | 1.00 | 53.24 | A | N |
| MOTA | 590 | CA | GLY | A | 198 | 261.296 | -63.164 | 92.148 | 1.00 | 47.33 | A | C |
| ATOM | 591 | C | | | 198 | | -63.697 | 93.360 | | 48.93 | A | |
| ATOM | 592 | Ö | | | 198 | | -63.928 | 94.412 | | 49.80 | A | |
| ATOM | 593 | N | | | 199 | | -63.941 | 93.204 | | 48.77 | A | |
| ATOM | 594 | CA | | | 199 | | -64.436 | 94.315 | | 50.98 | A | |
| | 595 | CB | | | | | -65.834 | | | | | |
| ATOM | | | | | 199 | | | 94.699 | | 54.11 | A | |
| ATOM | 596 | CG | | | 199 | | -66.921 | 93.853 | | 56.57 | A | |
| MOTA | 597 | CD1 | | | 199 | | -67.521 | 94.238 | | 57.21 | A | |
| ATOM | 598 | | TYR | | | | -68.526 | 93.471 | 1.00 | 58.18 | A | . C |
| ATOM | 599 | | TYR | | | | -67.351 | 92.664 | | 59.67 | A | |
| ATOM | 600 | | TYR | | | | -68.349 | 91.899 | | 59.17 | A | C |
| MOTA | 601 | CZ | | | 199 | | -68.933 | 92.308 | 1.00 | 59.36 | A | C |
| ATOM | 602 | OH | TYR | A | 199 | 266.075 | -69.917 | 91.535 | 1.00 | 63.54 | A | . 0 |
| ATOM | 603 | С | TYR | Α | 199 | 265.563 | -64.463 | 93.826 | 1.00 | 48.41 | A | C |
| ATOM | 604 | 0 | TYR | Α | 199 | 265.787 | -64.357 | 92.640 | 1.00 | 47.41 | A | . 0 |
| MOTA | 605 | N | PHE | Α | 200 | 266.542 | -64.591 | 94.701 | 1.00 | 43.25 | A | N |
| ATOM | 606 | CA | PHE | Α | 200 | | -64.582 | 94.221 | | 40.67 | A | |
| ATOM | 607 | СВ | | | 200 | | -63.159 | 93.950 | | 43.34 | A | |
| MOTA | 608 | CG | | | 200 | | -62.218 | 95.134 | | 48.79 | A | |
| ATOM | 609 | | PHE | | | | -62.115 | 96.166 | | 50.06 | A | |
| | 610 | | PHE | | | | -61.322 | 95.162 | | | | |
| ATOM | | | PHE | | | | | | | 52.88 | A | |
| ATOM | 611 | | | | | | -61.097 | 97.192 | | 53.41 | A | |
| ATOM | 612 | | PHE | | | | -60.331 | 96.166 | | 49.85 | A | |
| ATOM | 613 | CZ | | | 200 | | -60.201 | 97.160 | | 49.27 | A | |
| MOTA | 614 | С | | | 200 | | -65.113 | 95.325 | | 47.09 | A | |
| ATOM | 615 | 0 | | | 200 | 268.037 | -65.599 | 96.262 | 1.00 | 47.13 | A | 0 |
| MOTA | 616 | N | HIS | Α | 201 | 269.953 | -65.125 | 95.219 | 1.00 | 56.46 | A | N |
| ATOM | 617 | CA | HIS | Α | 201 | 270.635 | -65.604 | 96.382 | 1.00 | 56.94 | Α | С |
| ATOM | 618 | CB | HIS | A | 201 | 270.242 | -67.052 | 96.679 | 1.00 | 62.89 | А | |
| ATOM | 619 | CG | | | 201 | | -68.030 | 95.648 | | 66.27 | A | |
| ATOM | 620 | | HIS | | | | -68.454 | 94.469 | | 68.86 | A | |
| ATOM | 621 | | HIS | | | | -68.658 | 95.778 | | 70.42 | A | |
| ATOM | 622 | | HIS | | | | -69.425 | 94.727 | | 63.77 | A | |
| AT OF | 022 | CE T | TITO | 22 | 201 | 212.000 | - 07.423 | 23.161 | 1.00 | 03.11 | A | C |

| ATOM | 623 | | HIS | | | 271.048 | -69.319 | 93.917 | 1.00 | 69.53 | | A | N |
|--------------|------------|--------|------------|---|------------|---------|--------------------|------------------|------|----------------|---|----------|--------|
| ATOM | 624 | С | HIS | | | | -65.339 | 96.531 | 1.00 | 59.01 | | A | С |
| ATOM | 625 | 0 | HIS | | | | -64.604 | 95.737 | 1.00 | 56.46 | | A | 0 |
| ATOM | 626 | N | ASP | | | | -65.783 | 97.652 | | 53.50 | | A | N |
| ATOM | 627 | CA | ASP | | | | -65.546 | 97.850 | | 58.12 | | A | С |
| ATOM | 628 | CB | | | 202 | | -64.225 | 98.617 | | 61.13 | | A | С |
| ATOM | 629 | CG | | | 202 | | -64.255 | | | 65.37 | | A | С |
| ATOM | 630 | | ASP | | | | -65.308 | | | 69.09 | | A. | 0 |
| ATOM | 631 | | ASP | | | | -63.181 | | | 73.25 | | A | 0 |
| ATOM ATOM | 632 633 | С 0 | | | 202 202 | | -66.745 -67.899 | 98.522 | | 59.73 | | A | С |
| ATOM | 634 | И | | | 202 | | -66.473 | 98.426 99.163 | | 61.93 59.60 | | A. | 0 |
| ATOM | 635 | CA | | | 203 | | -67.507 | 99.793 | | 59.80 | | A | С И |
| ATOM | 636 | CB | | | 203 | | -66.933 | | | 57.31 | | A A | C |
| ATOM | 637 | C | | | 203 | | -68.138 | | | 60.08 | | A A | c |
| ATOM | 638 | ō | | | 203 | | -69.294 | | | 62.79 | | A | Ö |
| ATOM | 639 | N | | | 204 | | -67.377 | | | 60.13 | | A | N |
| ATOM | 640 | CA | THR | A | 204 | | -67.893 | | | 58.14 | | A | Ċ |
| MOTA | 641 | CB | THR | A | 204 | | -67.010 | | | 54.92 | | A | Č |
| ATOM | 642 | OG1 | THR | A | 204 | | -65.622 | | 1.00 | 51.82 | | A | Ó |
| ATOM | 643 | CG2 | THR | A | 204 | 276.406 | -67.388 | 104.681 | 1.00 | 55.25 | | Α | С |
| ATOM | 644 | С | THR | A | 204 | 273.203 | -68.070 | 102.993 | 1.00 | 61.74 | | A | С |
| MOTA | 645 | 0 | | | 204 | | -69.063 | | 1.00 | 66.23 | | A | Ο. |
| ATOM | 646 | N | | | 205 | | -67.099 | | 1.00 | 58.56 | | A | N |
| ATOM | 647 | CA | | | 205 | | -67.217 | | | 58.96 | | A | С |
| ATOM | 648 | CB | | | 205 | | -66.287 | | | 56.07 | | A | С |
| ATOM | 649 | CG | | | 205 | | -64.877 | | | 59.74 | | A | С |
| ATOM | 650 | CD | | | 205 | | -64.493 | | | 62.84 | | A | С |
| ATOM | 651 | NE | | | 205 | | -63.462 | | | 73.59 | | A | N |
| MOTA | 652 653 | CZ | | | 205 | | -62.747 | | | 79.55 | | A | C |
| ATOM ATOM | 654 | | ARG ARG | | | | -62.946 -61.845 | | | 80.70 | | A | N |
| ATOM | 655 | C | | | 205 | | -67.012 | | | 87.21 | | A. | И |
| MOTA | 656 | Ö | | | 205 | | -66.604 | | | 56.37 64.50 | | A A | С 0 |
| ATOM | 657 | N | | | 206 | | -67.373 | | | 54.49 | | A | И |
| ATOM | 658 | CA | | | 206 | | -67.238 | 99.960 | | 50.29 | | A. | C |
| ATOM | 659 | CB | | | 206 | | -68.522 | 99.670 | | 47.01 | | A | č |
| ATOM | 660 | CG1 | VAL | Α | 206 | | -68.370 | 98.374 | | 38.39 | | A | Č |
| ATOM | 661 | CG2 | VAL | A | 206 | 268.488 | -69.696 | 99.620 | | 42.93 | | A | C |
| ATOM | 662 | С | VAL | A | 206 | 267.306 | -66.124 | 100.321 | 1.00 | 50.23 | | A | С |
| ATOM | 663 | 0 | VAL | A | 206 | 266.870 | -65.982 | 101.487 | 1.00 | 49.82 | | Α | 0 |
| ATOM | 664 | N | | | 207 | | -65.330 | 99.320 | 1.00 | 47.64 | | Α | N |
| ATOM | 665 | CA | | | 207 | | -64.226 | 99.517 | 1.00 | 47.19 | | A | С |
| ATOM | 666 | CB | | | 207 | | -62.879 | 99.204 | | 44.49 | | A | С |
| ATOM | 667 | CG | | | 207 | | -62.684 | 99.852 | | 52.24 | | A | С |
| ATOM | 668 | CD1 | | | 207 | | -63.362 | 99.385 | | 51.97 | | A | C |
| ATOM | 669 670 | | TYR TYR | | | 2/0.438 | -63.194 -61.820 | 99.978 | | 60.89 | | A | C |
| ATOM ATOM | 671 | | TYR | | | | -61.638 | | | 55.49 | | A | C |
| ATOM | 672 | CZ | | | 207 | | -62.327 | | | 62.31 60.88 | | A | C |
| ATOM | 673 | OH | | | 207 | | -62.141 | | | 68.24 | | A A | C |
| ATOM | 674 | C | | | 207 | | -64.374 | 98.618 | | 42.31 | | A | C |
| ATOM | 675 | Õ | | | 207 | | -64.704 | 97.438 | | 43.03 | | A | ŏ |
| ATOM | 676 | N | LEU | A | 208 | | -64.078 | 99.171 | | 47.18 | | A | Ŋ |
| ATOM | 677 | CA | LEU | Α | 208 | | -64.129 | 98.377 | | 49.66 | | A | C |
| MOTA | 678 | CB | LEU | A | 208 | 261.411 | -65.084 | 99.005 | 1.00 | 50.68 | | A | С |
| ATOM | 679 | CG | LEU | A | 208 | 261.731 | -66.573 | 98.967 | | 50.97 | | A | С |
| ATOM | 680 | | LEU | | | | -67.349 | 99.471 | 1.00 | 51.61 | | A | С |
| ATOM | 681 | | LEU | | | | -66.964 | 97.575 | | 53.77 | | A | С |
| MOTA | 682 | С | | | 208 | | -62.733 | 98.264 | | 50.25 | | A | С |
| ATOM | 683 | 0 | | | 208 | | -62.085 | 99.278 | | 54.78 | | A. | 0 |
| ATOM | 684 | N | | | 209 | | -62.286 | 97.027 | | 50.37 | | A. | N |
| ATOM | 685 | CA | | | 209 | | -60.971 | 96.752 | | 49.74 | | A | C |
| ATOM | 686 687 | CB | ILE | | 209 | | -60.499 | 95.420 | | 50.44 | | A | С |
| ATOM ATOM | 688 | | ILE | | | | -59.096 -60.485 | 95.082 | | 50.97 | | A. | С |
| ATOM | 689 | | ILE | | | | -60.607 | 95.511 94.181 | | 49.66 51.66 | | A. | C |
| ATOM | 690 | CDI | | | 209 | | -61.075 | 96.749 | | 51.66 | | A A | C C |
| ATOM | 691 | o | | | 209 | | -61.543 | 95.755 | | 54.45 | | A. A. | 0 |
| ATOM | 692 | N | | | 210 | | -60.655 | 97.854 | | 47.03 | | A. | N |
| | | -• | | | | | | | | | • | • • | -4 |

| ATOM | 693 | CA | LEU | А | 210 | 25 | 7.53 |) -6 | 729 | 2 | 7.990 | 7 (| ١٥ | 43.40 | 70 | ~ |
|------|-----|-----|-------|---|-----|-----|-------|-------|-------|------|-------|------|-----|-------|----|---|
| ATOM | 694 | CB | | | 210 | | | | | | | | | | A | C |
| | | | | | | | 7.16 | | | | 9.362 | | | 43.91 | A | С |
| MOTA | 695 | CG | | | 210 | | 7.76 | | | | 9.773 | 1.0 | 00 | 42.46 | Α | C |
| ATOM | 696 | | LEU | | | 25 | 7.69 | 5 -62 | 2.764 | 10: | 1.264 | 1.0 | 00 | 44.44 | Α | C |
| MOTA | 697 | CD2 | LEU | Α | 210 | 25 | 7.02 | 9 -63 | 3.701 | . 99 | 9.100 | 1.0 | 00 | 44.23 | Α | С |
| ATOM | 698 | С | LEU | Α | 210 | | 6.87 | | | | 7.827 | | | 42.69 | A | č |
| MOTA | 699 | 0 | | | 210 | | 7.52 | | | | | | | | | |
| ATOM | 700 | Ŋ | | | | | | | | | 7.627 | | | 50.83 | A | 0 |
| | | | | | 211 | | 5.55 | | | | 7.901 | 1.0 | 00 | 45.93 | Α | N |
| MOTA | 701 | CA | | | 211 | | 4.75 | | | | 7.813 | 1.0 | 00 | 41.90 | A | С |
| ATOM | 702 | CB | GLU | A | 211 | 25 | 3.38: | 3 -58 | 3.471 | . 97 | 7.201 | 1.0 | 00 | 39.85 | A | С |
| MOTA | 703 | CG | GLU | Α | 211 | 25 | 2.40 | 2 -5 | 7.354 | 91 | 7.290 | | | 41.17 | A | Č |
| ATOM | 704 | CD | GLU | Α | 211 | | 0.97 | | | | 5.890 | | | 51.54 | | č |
| ATOM | 705 | | GLU | | | | 0.012 | | | | | | | - | A | |
| ATOM | 706 | | GLU | | | | | | | | 7.025 | | | 57.54 | A | 0 |
| | | | | | | | 0.79 | | | | 5.438 | | | 52.59 | A | 0 |
| MOTA | 707 | С | | | 211 | | 4.608 | | | | 9.259 | 1.0 | 00 | 38.67 | Α | С |
| ATOM | 708 | 0 | GLU | A | 211 | 25 | 4.50 | 7 -58 | 3.477 | 100 | 200 | 1.0 | 00 | 42.39 | A | 0 |
| MOTA | 709 | N | TYR | Α | 212 | 25 | 4.619 | 9 -56 | 5.346 | 99 | 9.428 | 1.0 | 00 | 43.63 | A | N |
| ATOM | 710 | CA | TYR | Α | 212 | | | | | | 757 | | | 47.96 | A | Ĉ |
| ATOM | 711 | CB | | | 212 | | | | | | 7.753 | | | | | |
| ATOM | 712 | CG | | | 212 | | | | | | | | | 46.03 | A | C |
| | | | | | | | | | | | 2.025 | | | 44.95 | A | С |
| ATOM | 713 | | TYR | | | | | | | | 3.259 | 1.0 | 00 | 42.54 | A | С |
| MOTA | 714 | | TYR | | | | | | | | 1.429 | 1.0 | 0 | 48.54 | Α | С |
| ATOM | 715 | CD2 | TYR | Α | 212 | 25 | 4.639 | 9 -52 | 2.193 | 101 | L.984 | 1.0 | 00 | 44.86 | A | C |
| ATOM | 716 | CE2 | TYR | Α | 212 | | | | | | 3.164 | | | 50.04 | A | Ċ |
| ATOM | 717 | CZ | | | 212 | | | | | | 1.372 | | | 48.45 | | |
| ATOM | 718 | OH | | | 212 | | 4.523 | | | | | | | | A | C |
| ATOM | 719 | C | | | 212 | | | | | | | | | 53.45 | A | 0 |
| | | | | | _ | | | | | | .248 | | | 50.57 | Α | С |
| ATOM | 720 | 0 | | | 212 | | 2.153 | | | | | 1.0 | 0 | 51.02 | A | 0 |
| ATOM | 721 | N | ALA | A | 213 | | 2.799 | | | | | 1.0 | 0 | 48.23 | A. | N |
| MOTA | 722 | CA | ALA | A | 213 | 25 | 1.459 | -56 | 5.040 | 103 | 3.078 | 1.0 | 0 | 51.96 | A | C |
| ATOM | 723 | CB | ALA | Α | 213 | | 1.084 | | | | | | | 42.77 | A | č |
| ATOM | 724 | С | ALA | | | 25 | 1.528 | -54 | 973 | 104 | 177 | | | 46.25 | | |
| ATOM | 725 | ō | | | 213 | | 1.958 | | | | | | | | A. | C |
| ATOM | 726 | И | | | | | | | | | | | | 57.39 | A | 0 |
| | | | PRO | | | | 1.109 | | | | | 1.0 | 0 | 45.44 | Α | N |
| ATOM | 727 | CD | PRO | | | | 0.592 | | | | | 1.0 | 0 | 45.81 | A | С |
| ATOM | 728 | CA | PRO | А | 214 | | 1.118 | | | | | 1.0 | 0 | 37.64 | Α | С |
| MOTA | 729 | CB | PRO | Α | 214 | 25 | 0.400 | -51 | .512 | 103 | .991 | | | 44.41 | A | Ċ |
| ATOM | 730 | CG | PRO | Α | 214 | | 0.755 | | | | | | | 45.51 | A | č |
| ATOM | 731 | С | PRO | | | | 0.481 | | | | | | | 39.63 | | |
| ATOM | 732 | ō | PRO | | | | 1.116 | | | | | | | | A | С |
| ATOM | 733 | N | LEU | | | | | | | | | | | 38.67 | Ą | 0 |
| ATOM | | | | | | | 9.287 | | | | | | | 33.01 | A | N |
| | 734 | CA | LEU | | | | 8.570 | | | | | | | 35.54 | A | С |
| ATOM | 735 | CB | LEU | | | | 7.074 | | | | | 1.0 | 0 | 39.80 | A | С |
| ATOM | 736 | CG | LEU | A | 215 | 24 | 6.571 | 52 | .332 | 106 | .331 | 1.0 | 0 | 39.22 | A | C |
| ATOM | 737 | CD1 | LEU | A | 215 | 24 | 5.025 | -52 | .236 | 106 | . 407 | | | 37.56 | A | č |
| ATOM | 738 | | LEU | | | 24 | 7.156 | -51 | 166 | 106 | ROR | | | 36.39 | | |
| MOTA | 739 | С | LEU | | | 24 | 8.923 | -54 | 905 | 100 | 240 | | _ | | A | C |
| ATOM | 740 | ō | LEU | | | 24 | 0.323 | - 54 | 100 | 100 | . 240 | | | 43.21 | A | С |
| | | | | | | 24 | 8.208 | -55 | . 121 | 109 | .220 | | | 39.03 | Α | 0 |
| ATOM | 741 | N | GLY | | | 25 | 0.022 | -55 | .466 | 107 | .906 | | | 42.62 | A | N |
| ATOM | 742 | CA | GLY | | | 25 | 0.443 | -56 | .630 | 108 | .669 | 1.0 | 0 | 46.42 | A | С |
| ATOM | 743 | С | GLY | | | 24 | 9.594 | -57 | .891 | 108 | .554 | 1.0 | 0 | 44.15 | A | С |
| MOTA | 744 | 0 | GLY | A | 216 | 24 | 8.995 | -58 | .166 | 107 | .504 | | | 46.45 | A | ō |
| ATOM | 745 | N | THR | | | 24 | 9.523 | -58 | . 640 | 109 | 656 | | | 39.98 | | |
| ATOM | 746 | CA | THR | | | 24 | 3.774 | -50 | 888 | 100 | 660 | | | | A | N |
| ATOM | 747 | СВ | THR | | | 241 | 3 602 | 61 | 040 | 110 | .005 | | | 43.21 | A | С |
| ATOM | | | THR | | | 24 | 9.583 | -01 | .040 | 110 | .286 | | | 43.67 | A | С |
| | 748 | | | | | 24 | 9.791 | -60 | . 782 | 111 | .678 | | | 51.00 | A | 0 |
| ATOM | 749 | | THR | | | | 0.905 | | | | | 1.0 | 0 | 41.04 | A | С |
| ATOM | 750 | С | THR | Ą | 217 | 24' | 7.450 | -59 | .858 | 110 | .416 | 1.0 | 0 4 | 42.99 | A | С |
| MOTA | 751 | 0 | THR | Α | 217 | 24' | 7.185 | -58 | .962 | 111 | .227 | | | 41.59 | A | ŏ |
| ATOM | 752 | N | VAL | | | 241 | 5.646 | -60 | .881 | 110 | . 166 | | | 41.73 | A | |
| ATOM | 753 | CA | VAL | | | 24 | 3.335 | -61 | 037 | 110 | 766 | | | | | N |
| ATOM | 754 | CB | VAL | | | | | | | | | | | 41.12 | A | C |
| | | | | | | 244 | 1.564 | -02 | .091 | 109 | .9/0 | | | 41.84 | A | С |
| MOTA | 755 | | VAL . | | | | 3.170 | | | | | 1.0 | 0 4 | 43.61 | Α | С |
| ATOM | 756 | | VAL . | | | | 1.544 | | | | | | | 33.71 | A | С |
| MOTA | 757 | С | VAL . | Α | 218 | 245 | 6.610 | -61 | .486 | 112 | .201 | | | 40.94 | A | Ċ |
| ATOM | 758 | 0 | VAL . | A | 218 | 244 | .789 | -61 | .326 | 113 | .078 | | | 51.00 | A | ŏ |
| ATOM | 759 | N | TYR . | | | | .801 | | | | | | | 15.88 | A | |
| ATOM | 760 | CA | TYR | | | 247 | .233 | -62 | 494 | 112 | 757 | | | 12.54 | | N |
| ATOM | 761 | CB | TYR : | | | | .607 | | | | | | | | A | C |
| | | | | | | | | | | | | | | 15.91 | A | С |
| ATOM | 762 | CG | TYR . | A | Z13 | 245 | .102 | -63 | .0/6 | 115 | .011 | 1.00 |) 4 | 16.80 | A | С |

| ATOM | 763 | CD1 | TYR | Α | 219 | 248,755 | -64.925 | 115.464 | 1.00 | 45.83 | | A | С |
|------|-----|------|-------------|-----|-------|---------|---------|---------|------|-------|---|------------|---|
| | | | | | | | | | | | | | |
| ATOM | 764 | | TYR | | | | -65.377 | | 1.00 | 53.23 | 4 | 4 | С |
| ATOM | 765 | CD2 | TYR | Α | 219 | 249.884 | -62.892 | 115.825 | 1.00 | 46.38 | | J. | С |
| MOTA | 766 | | TYR | | | | | | | | | | |
| | | | | | | | -63.314 | | | 52.61 | 4 | | С |
| ATOM | 767 | CZ | TYR | A | 219 | 249.961 | -64.565 | 117.510 | 1.00 | 53.76 | | A. | С |
| ATOM | 768 | OH | TYR | Δ | 219 | 250.361 | -64.985 | 118 789 | 1 00 | 54.10 | | A | 0 |
| | | | | | | | | | | | | | |
| ATOM | 769 | С | TYR | А | 219 | 247.323 | -61.287 | 114.702 | 1.00 | 44.93 | 1 | £ | С |
| MOTA | 770 | 0 | TYR | Α | 219 | 246.745 | -61.322 | 115.825 | 1.00 | 40.09 | | A. | 0 |
| | | | | | | | | | | | | | |
| ATOM | 771 | N | ARG | А | 220 | 248.031 | -60.243 | 114.240 | 7.00 | 37.14 | 4 | A | N |
| ATOM | 772 | CA | ARG | Α | 220 | 248.172 | -59.035 | 115.029 | 1.00 | 44.63 | | A. | С |
| ATOM | 773 | CB | ARG | л | 220 | 2/0 213 | -58.086 | 11/ 206 | | 42.95 | | | C |
| | | | | | | | | | | | | | |
| MOTA | 774 | С | ARG | A | 220 | 246.828 | -58.318 | 115.225 | 1.00 | 43.95 | | A | С |
| ATOM | 775 | 0 | ARG | Δ | 220 | 246.563 | -57.773 | 116 314 | 1 00 | 44.55 | | A. | 0 |
| | | | | | | | | | | | | | |
| ATOM | 776 | N | GLU | A | 221 | 245.973 | -58.369 | 114.198 | T.00 | 44.85 | | A. | N |
| MOTA | 777 | CA | GLU | Α | 221 | 244.688 | -57.692 | 114.255 | 1.00 | 43.30 | | A | С |
| ATOM | 778 | CB | GLU | 70 | 221 | 244 031 | -57.678 | 112 004 | | 46.86 | | | С |
| | | | | | | | | | | | | | |
| ATOM | 779 | CG | GLU | A | 221 | 242.921 | -56.648 | 112.713 | 1.00 | 56.65 | | A | С |
| ATOM | 780 | CD | GLU | А | 221 | 243.442 | -55.193 | 112.758 | 1.00 | 63.09 | | A | С |
| | | | | | | | -54.238 | | | | | | |
| MOTA | 781 | | GLU | | | | | | 1.00 | 66.10 | | A | 0 |
| ATOM | 782 | OE2 | GLU | Α | 221 | 244.670 | -55.005 | 112.919 | 1.00 | 66.07 | | A. | 0 |
| ATOM | 783 | С | GLÜ | ΖΔ. | 221 | 243 806 | -58.412 | 115 243 | 1 00 | 46.56 | | A. | С |
| | | | | | | | | | | | | | |
| ATOM | 784 | 0 | GTO | A | 221 | 242.959 | -57.802 | 115.900 | 1.00 | 44.66 | | A | 0 |
| MOTA | 785 | N | LEU | Α | 222 | 244.028 | -59.719 | 115.362 | 1.00 | 46.74 | | A | N |
| | | | | | | | -60.550 | | | | | | |
| ATOM | 786 | CA | LEU | | | | | | | 40.98 | | | С |
| ATOM | 787 | CB | LEU | Α | 222 | 243.444 | -62.013 | 115.880 | 1.00 | 42.79 | | Ą | С |
| ATOM | 788 | CG | USLI | Δ | 222 | 242 339 | -62.985 | 116 313 | 1 00 | 48.20 | | A | С |
| | | | | | | | | | | | | | |
| atom | 789 | | $_{ m LEU}$ | | | | -62.509 | | 1.00 | 42.35 | | | С |
| ATOM | 790 | CD2 | LEU | A | 222 | 242.649 | -64.361 | 115.761 | 1.00 | 47.96 | | A | С |
| ATOM | 791 | С | T.WIT | 7 | 222 | 2/3 7// | -60.292 | 117 710 | | 45.64 | | | C |
| | | | | | | | | | | | | | |
| MOTA | 792 | 0 | LEU | Α | 222 | 242.995 | -60.390 | 118.692 | 1.00 | 46.35 | | Ą | 0 |
| ATOM | 793 | N | GLN | Α | 223 | 245,008 | -59.938 | 117.875 | 1.00 | 47.19 | | A | N |
| | | | | | 223 | | | | | | | | |
| ATOM | 794 | CA | | | | | -59.670 | | | 48.16 | | | С |
| ATOM | 795 | CB | GLN | А | 223 | 247.056 | -59.584 | 119.112 | 1.00 | 49.22 | | A | С |
| MOTA | 796 | CG | GT.N | Δ | 223 | 247 819 | -60.926 | 119.032 | 1 00 | 56.96 | | A | С |
| | | | | | | | | | | | | | |
| ATOM | 797 | CD | GLIN | A | 223 | | -60.732 | | 1.00 | 66.12 | | A | С |
| ATOM | 798 | OE1 | GLN | A | 223 | 249.807 | -59.935 | 117.981 | 1.00 | 68.93 | | A | 0 |
| ATOM | 799 | ME 2 | GLN | Δ | 223 | 250 067 | -61.453 | 110 755 | | 65.96 | | | N |
| | | | | | | | | | | | | | |
| ATOM | 800 | С | GLN | Α | 223 | 244.994 | -58.332 | 119.711 | 1.00 | 54.79 | | A | С |
| ATOM | 801 | 0 | GLN | Α | 223 | 244.710 | -58.153 | 120.899 | 1.00 | 63.31 | | A | 0 |
| | 802 | N | | | 224 | | -57.398 | | | | | | |
| ATOM | | | | | | | | | | 53.43 | | | N |
| MOTA | 803 | CA | LYS | Α | 224 | 244.412 | -56.042 | 119.021 | 1.00 | 52.16 | | Ą | С |
| ATOM | 804 | CB | LYS | Α | 224 | 244.668 | -55.276 | 117,729 | 1.00 | 51.41 | | A | С |
| | - | | | | | | | | | | | | |
| ATOM | 805 | CG | | | 224 | | -53.805 | | 1.00 | 58.82 | | A | С |
| ATOM | 806 | CD | LYS | A | 224 | 245.109 | -53.234 | 116.429 | 1.00 | 58.34 | | A | С |
| ATOM | 807 | CE | 7.79 | Δ | 224 | 244 105 | -52.175 | 115 057 | | 57.11 | | | C |
| | | | | | | | | | | | | | |
| ATOM | 808 | NZ | LYS | A | 224 | 243.509 | -52.549 | 114.632 | | 62.05 | | A | N |
| ATOM | 809 | С | LYS | A | 224 | 242.909 | -55.999 | 119.415 | 1.00 | 46.25 | | A | С |
| ATOM | 810 | 0 | | | 224 | | -55.374 | | | 53.53 | | | |
| | | | | | | | | | | | | | 0 |
| MOTA | 811 | N | TEO | A | 225 | | | 118.658 | | 40.03 | | A | N |
| ATOM | 812 | CA | LEU | Α | 225 | 240.616 | -56.712 | 118.885 | 1.00 | 28.18 | | A | С |
| | 813 | CB | | | 225 | | -56.682 | | | | | | |
| ATOM | | | | | | | | | | 32.03 | | | С |
| ATOM | 814 | CG | LEU | A | 225 | 240.538 | -55.704 | 116.515 | 1.00 | 37.72 | | A . | С |
| ATOM | 815 | CD1 | LEU | Α | 225 | 239.725 | -55.736 | 115,208 | 1.00 | 28.64 | | Ą | С |
| | 816 | | LEU | | | | -54.252 | | | | | | |
| ATOM | | | | | | | | | | 32.47 | - | A. | С |
| ATOM | 817 | С | LEU | A | 225 | 240.076 | -57.907 | 119.686 | 1.00 | 39.70 | | 4 | С |
| ATOM | 818 | 0 | LEU | Α | 225 | 238.896 | -57.954 | 120.056 | 1.00 | 27.45 | | A | 0 |
| | | | | | | | | | | | | | |
| ATOM | 819 | N | SER | A | 226 | | | 119.958 | | 33.23 | 4 | A. | N |
| ATOM | 820 | CA | SER | Α | 226 | 240.528 | -60.051 | 120.695 | 1.00 | 38.91 | 1 | A. | С |
| ATOM | 821 | СВ | | | 226 | | | 122.015 | | 42.93 | | | č |
| | | | | | | | | | | | | | |
| MOTA | 822 | OG | | | 226 | | -58.570 | | | 59.01 | i | 4 | 0 |
| ATOM | 823 | С | SER | Α | 226 | 239.548 | -60.869 | 119.867 | 1.00 | 40.96 | 1 | Ŧ. | С |
| | 824 | | | | 226 | | -62.029 | | | | | | |
| ATOM | | 0 | | | | | | | | 45.01 | | | 0 |
| ATOM | 825 | N | LYS | A | 227 | 238.433 | -60.270 | 119.484 | 1.00 | 43.12 | 7 | 4 | N |
| ATOM | 826 | CA | | | 227 - | 237.409 | -60.968 | 118.693 | | 37.87 | | | С |
| | | | | | | | | | | | | | |
| ATOM | 827 | CB | | | 227 | | -61.246 | | | 41.34 | 1 | | С |
| ATOM | 828 | CG | LYS | Α | 227 | 236.384 | -62.150 | 120.650 | 1.00 | 49.95 | 1 | 4 | С |
| ATOM | 829 | CD | | | 227 | | -62.365 | | | 59.51 | | | Ċ |
| | | | | | | | | | | | | | |
| ATOM | 830 | CE | | | 227 | | -61.186 | | | 64.97 | 1 | | С |
| ATOM | 831 | NZ | LYS | Α | 227 | 234.813 | -61.628 | 123.907 | 1.00 | 64.50 | 1 | . . | N |
| | 832 | C | | | | | -60.044 | | | 37.96 | | | c |
| ATOM | 034 | C | nto | 4 | 227 | 231.009 | 00.044 | 111.520 | 1.00 | 37.30 | | A | · |

| | | | | - | ., | | | | | | |
|--------------|------------|-----------------|-------|--------------------|--------------------|--------------------|------|----------------|---|--------|--------|
| ATOM | 833 | O LYS A | 227 | 237.061 | -58.799 | 117.619 | 1.00 | 40.95 | | A | 0 |
| ATOM | 834 | N PHE A | | | | 116.431 | 1.00 | 34.94 | | A | N |
| MOTA | 835 | CA PHE A | | 236.175 | -59.917 | 115.262 | 1.00 | 34.74 | | A | C |
| ATOM | 836 | CB PHE A | | | | 113.998 | | 34.85 | | Α | C |
| ATOM | 837 | CG PHE A | | | | 113.849 | | 43.10 | | A | С |
| ATOM | 838 | CD1 PHE A | | | | 112.913 | | 43.37 | | A | C |
| MOTA | 839 | CD2 PHE A | | | | 114.656 | 1.00 | 38.38 | | A | С |
| ATOM | 840 | CE1 PHE A | | | | 112.796 | | 48.51 | | A | C |
| ATOM | 841 | CE2 PHE A | | 240.266 | -59.207 | 114.554 | | 47.20 | | Α | С |
| MOTA MOTA | 842 843 | CZ PHE A | | | | 113.631 | | 48.16 | | A | C |
| ATOM | 844 | C PHE A | | | | 115.208 | | 40.38 | | A | С |
| ATOM | 845 | N ASP A | | | | 115.664 | _ | 36.38 | | A | 0 |
| ATOM | 846 | CA ASP A | | | | 114.687 114.534 | | 40.55 38.86 | | A | N |
| ATOM | 847 | CB ASP A | | 231.823 | -57 832 | 114.334 | | 49.26 | | A | C |
| ATOM | 848 | CG ASP A | | 232.394 | -56.912 | 113.357 | | 51.97 | | A A | C |
| ATOM | 849 | OD1 ASP A | | | | 112.179 | | 54.02 | | A | 0 |
| ATOM | 850 | OD2 ASP A | | | | 113.699 | | 55.60 | | A | o |
| MOTA | 851 | C ASP A | | | | 113.304 | | 41.70 | | A | c |
| ATOM | 852 | O ASP A | 229 | | | 112.480 | | 35.62 | | A | ŏ |
| ATOM | 853 | N GLU A | | 230.905 | ~60.365 | 113.193 | | 40.43 | | A | N |
| MOTA | 854 | CA GLU A | | 230.434 | -61.213 | 112.114 | 1.00 | 43.61 | | A | C |
| ATOM | 855 | CB GLU A | | | | 112.298 | 1.00 | 43.33 | | A | С |
| ATOM | 856 | CG GLU A | | | | 113.653 | 1.00 | 43.90 | | A | С |
| ATOM | 857 | CD GLU A | | 227.292 | -62.967 | 113.627 | 1.00 | 48.51 | | Α | С |
| MOTA | 858 | OE1 GLU A | | | | 113.308 | | 37.93 | | A | 0 |
| ATOM | 859 | OE2 GLU A | | 227.300 | -64.204 | 113.916 | | 42.11 | | A | 0 |
| ATOM ATOM | 860 861 | C GLU A O GLU A | | | | 110.778 | | 43.16 | | A | С |
| ATOM | 862 | N GLN A | | | | 109.779 | | 50.29 | | A | 0 |
| ATOM | 863 | CA GLN A | | | | 110.748 109.489 | | 49.18 | | A | N |
| ATOM | 864 | CB GLN A | | | | 109.485 | | 49.70 57.14 | | A | C |
| ATOM | 865 | CG GLN A | | 229.958 | -56.236 | 108.412 | 1 00 | 62.54 | | A A | C |
| ATOM | 866 | CD GLN A | | 231.200 | -55.770 | 107.642 | | 71.69 | | A A | C |
| ATOM | 867 | OE1 GLN A | | 232.065 | -55.042 | 108.191 | | 72.68 | | A | o |
| ATOM | 868 | NE2 GLN A | . 231 | | | 106.359 | | 72.33 | | A | И |
| MOTA | 869 | C GLN A | . 231 | 232.197 | | | | 45.76 | | A | C |
| MOTA | 870 | O GLN A | | 232.470 | -58.874 | 107.846 | | 46.46 | | A | 0 |
| ATOM | 871 | N ARG A | | 233.131 | -58.437 | 109.949 | | 43.95 | | A | N |
| ATOM | 872 | CA ARG A | | 234.560 | | | | 38.33 | | A | C |
| ATOM ATOM | 873 874 | CB ARG A | | 235.365 | -57.998 | 110.861 | | 39.16 | | A | С |
| ATOM | 875 | CD ARG A | | 236.867 237.514 | -58.073 | 110.703 | | 31.46 | | A | С |
| MOTA | 876 | NE ARG A | | 237.314 | -56 Q15 | 111 224 | | 51.25 | | A. | С |
| ATOM | 877 | CZ ARG A | | 239.275 | | | | 58.24 65.45 | | A. | N |
| ATOM | 878 | NH1 ARG A | | 238.395 | -54.594 | 111.226 | 1.00 | 62.45 | | A A | C N |
| ATOM | 879 | NH2 ARG A | 232 | 240.551 | -55.369 | 110.780 | | 72.17 | | a A | |
| MOTA | 880 | C ARG A | | 234.950 | -59.946 | 109.369 | | 42.02 | | A. | С |
| ATOM | 881 | O ARG A | 232 | 235.757 | -60.183 | 108.517 | | 45.04 | | A | õ |
| ATOM | 882 | N THR A | | 234.372 | | | 1.00 | 43.50 | | A | Ŋ |
| MOTA | 883 | CA THR A | | 234.697 | -62.320 | 109.891 | | 37.00 | | Ą | C |
| MOTA | 884 | CB THR A | | 234.104 | -63.175 | 110.992 | | 35.89 | | A. | C |
| ATOM | 885 | OG1 THR A | | 234.543 | -62.696 | 112.268 | | 30.74 | | A | 0 |
| ATOM | 886 | CG2 THR A | | 234.488 | -64.641 | 110.763 | | 22.73 | | A | С |
| ATOM ATOM | 887 888 | C THR A O THR A | | 234.149 | | | 1.00 | 45.73 | | A | С |
| ATOM | 889 | N ALA A | | 234.857 232.892 | | | 1.00 | 45.99 | | A | 0 |
| ATOM | 890 | CA ALA A | | 232.256 | | | 1.00 | 44.83 | | A. | N |
| MOTA | 891 | CB ALA A | | 230.852 | -62.837 -62.351 | 106.960 | | 41.77 39.48 | | Ą | C |
| ATOM | 892 | C ALA A | | 233.064 | | | | 44.77 | | A A | C C |
| ATOM | 893 | O ALA A | | 233.273 | | | | 39.69 | | A A | 0 |
| ATOM | 894 | N THR A | 235 | 233.543 | | | | 43.07 | | i. | N |
| MOTA | 895 | CA THR A | | 234.328 | | | 1.00 | 44.31 | | Ä | C |
| ATOM | 896 | CB THR A | 235 | 234.557 | -59.058 | 104.926 | | 44.88 | | Ä | Ċ |
| ATOM | 897 | OG1 THR A | | 233.306 | -58.373 | 104.984 | | 49.29 | | 4 | ŏ |
| ATOM | 898 | CG2 THR A | | 235.343 | | | | 37.93 | Į | | C |
| ATOM | 899 | C THR A | | 235.689 | | | 1.00 | 47.59 | Į | | C |
| ATOM | 900 | O THR A | | 236.169 | | | | 49.69 | Į | 1 | 0 |
| ATOM | 901 | N TYR A | | 236.310 | | | | 47.35 | F | 1 | N |
| ATOM | 902 | CA TYR A | 236 | 237.613 | -62.189 | 105.850 | 1.00 | 46.90 | P | 7 | С |
| | | | | | | | | | | | |

18/73 ATOM 903 CB TYR A 236 238.206 -62.221 107.255 1.00 42.67 MOTA 904 CG TYR A 236 239.024 -61.003 107.621 1.00 45.24 С ATOM 905 CD1 TYR A 236 239.154 -59.930 106.767 1.00 40.32 239.909 -58.819 107.134 1.00 51.10 MOTA 906 CE1 TYR A 236 Α С ATOM 907 CD2 TYR A 236 239.667 -60.929 108.847 1.00 46.47 240.430 -59.808 109.228 1.00 52.60 Α С 908 CE2 TYR A 236 ATOM Α С CZ TYR A 236 240.542 -58.764 108.367 1.00 49.08 ATOM 909 С Α MOTA 910 OH TYR A 236 241.265 -57.653 108.719 1.00 58.26 0 Α ATOM 911 С TYR A 236 237.496 -63.604 105.334 1.00 47.98 Α 238.469 -64.148 104.832 1.00 58.71 236.296 -64.177 105.416 1.00 50.41 236.032 -65.540 104.944 1.00 46.45 TYR A 236 MOTA 912 0 A O ILE A 237 ATOM 913 N Α N MOTA 914 CA ILE A 237 Α С 234.816 -66.156 105.635 1.00 45.13 915 CB ILE A 237 MOTA Α С 234.357 -67.442 104.903 1.00 42.23 235.157 -66.440 107.101 1.00 42.93 MOTA 916 CG2 ILE A 237 Α C CG1 ILE A 237 MOTA 917 Α C CD1 ILE A 237 236.253 -67.436 107.317 1.00 39.73 235.798 -65.597 103.462 1.00 51.53 MOTA 918 A C ILE A 237 919 MOTA С Α С 236.213 -66.548 102.822 1.00 55.68 MOTA 920 0 ILE A 237 Α 0 MOTA 921 N THR A 238 235.148 -64.571 102.914 1.00 51.45 Α Ν 234.858 -64.526 101.471 1.00 44.65 922 CA THR A 238 MOTA A С 233.929 -63.346 101.106 1.00 44.82 232.653 -63.512 101.719 1.00 43.65 MOTA 923 CB THR A 238 С Α 924 OG1 THR A 238 MOTA Α 233.701 -63.294 99.660 1.00 44.50 MOTA 925 CG2 THR A 238 Α C MOTA 926 C THR A 238 236.166 -64.350 100.706 1.00 47.18 Α С 236.467 -65.090 99.782 1.00 48.37 236.956 -63.367 101.116 1.00 49.98 238.239 -63.082 100.473 1.00 52.23 ATOM 927 0 THR A 238 A 0 MOTA 928 N **GLU A 239** Α N CA GLU A 239 MOTA 929 Α С 238.937 -61.932 101.203 1.00 54.22 930 CB GLU A 239 MOTA Α C CG GLU A 239 MOTA 931 238.139 -60.624 101.260 1.00 55.95 Α С 238.811 -59.573 102.137 1.00 58.38 239.056 -59.843 103.333 1.00 65.65 239.099 -58.468 101.634 1.00 60.73 MOTA 932 CD GLU A 239 Α ATOM 933 OE1 GLU A 239 Α. O OE2 GLU A 239 934 MOTA Α 239.109 -64.330 100.496 1.00 50.02 MOTA 935 GLU A 239 C Α C 239.851 -64.616 99.561 1.00 55.72 MOTA 936 O GLU A 239 Α O 238.978 -65.104 101.557 1.00 49.14 239.768 -66.305 101.702 1.00 48.27 239.776 -66.717 103.173 1.00 46.82 LEU A 240 MOTA 937 N A. MOTA 938 CA LEU A 240 A С CB LEU A 240 MOTA 939 Α C 240.917 -67.581 103.679 1.00 45.79 MOTA 940 CG LEU A 240 Α С 242.225 -67.030 103.195 1.00 50.28 941 CD1 LEU A 240 ATOM Α C 240.885 -67.603 105.172 1.00 53.83 239.209 -67.420 100.833 1.00 49.65 239.960 -68.170 100.210 1.00 53.66 ATOM 942 CD2 LEU A 240 Α LEU A 240 MOTA 943 С Α C MOTA 944 0 LEU A 240 Α 237.883 -67.519 100.778 1.00 45.02 ATOM 945 N ALA A 241 Α N 946 CA ATOM ALA A 241 237.222 -68.549 99.965 1.00 50.04 Α C 235.724 -68.611 100.256 1.00 39.53 237.447 -68.278 98.481 1.00 47.71 CB 947 ALA A 241 MOTA Α C ATOM 948 С ALA A 241 Α C 237.495 -69.203 97.682 1.00 54.94 MOTA 949 0 ALA A 241 Α 0 MOTA 950 N ASN A 242 237.585 -67.012 98.114 1.00 49.50 A N 951 CA ASN A 242 MOTA 237.839 -66.637 96.729 1.00 51.78 Α С 952 CB **ASN A 242** 237.688 -65.134 96.554 1.00 45.48 ATOM A С 96.592 MOTA 953 CG ASN A 242 236.231 -64.680 1.00 51.39 A C 235.972 -63.489 96.769 1.00 50.23 MOTA 954 OD1 ASN A 242 Α 0 955 ND2 ASN A 242 MOTA 235.276 -65.620 96.412 1.00 43.58 Α N MOTA 956 С ASN A 242 239.241 -67.046 96.330 1.00 50.85 Α 239.419 -67.736 MOTA 957 0 **ASN A 242** 95.323 1.00 53.87 Α O 958 N ALA A 243 240.230 -66.625 MOTA 97.119 1.00 48.27 Α N 96.861 1.00 42.21 959 ALA A 243 241.629 -66.970 ATOM CA Α С MOTA 960 CB ALA A 243 242.534 -66.345 97.913 1.00 45.13 С A ALA A 243 MOTA 961 С 241.816 -68.473 96.880 1.00 43.95 A 1.00 42.43 MOTA 962 0 ALA A 243 242.498 -69.016 96.026 Α 0 241.219 -69.152 ATOM 963 N LEU A 244 97.858 1.00 40.59 A N 241.366 -70.606 97.945 1.00 48.68 ATOM 964 CA LEU A 244 Α C 965 240.689 ~71.141 ATOM CB LEU A 244 99.204 1.00 42.37 Α C 966 CG 241.465 -70.944 100.495 1.00 39.60 ATOM LEU A 244 Α C ATOM 967 CD1 LEU A 244 240.751 -71.763 101.602 1.00 37.99

242.889 -71.432 100.340

241.327 -72.330

N SER A 245 239.662 -70.777 96.200 1.00 61.51 CA SER A 245 239.010 -71.317 95.018 1.00 61.35

240.779 -71.311 96.702 1.00 56.87

CD2 LEU A 244

LEU A 244

LEU A 244

ATOM

MOTA

ATOM

ATOM

ATOM

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970

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972

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1.00 35.22

96.220 1.00 60.52

С

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0

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С

| ATOM | 973 | СВ | SER I | A 245 | 237.785 | -70.501 | 94.692 | 1.00 | 64.64 | A | . с |
|------|------|-----|-------|-------|---------|--------------------|--------|------|-------|------------|-----|
| ATOM | 974 | OG | | A 245 | | -70.779 | 93.390 | | 71.14 | A | |
| ATOM | 975 | C | | A 245 | | -71.242 | 93.855 | | 63.54 | | |
| MOTA | 976 | Ö | | A 245 | | -72.233 | | | | A | |
| | | | | | | | 93.134 | | 63.37 | <i>I</i> A | |
| ATOM | 977 | N | | A 246 | | -70.063 | 93.679 | | 58.29 | A | |
| ATOM | 978 | CA | | A 246 | | -69.855 | 92.633 | | 57.08 | A | |
| ATOM | 979 | CB | TYR . | A 246 | | -68.455 | 92.719 | 1.00 | 51.38 | A | C |
| MOTA | 980 | CG | TYR . | A 246 | 243.247 | -68.195 | 91.754 | 1.00 | 55.36 | , A | , C |
| ATOM | 981 | CD1 | TYR : | A 246 | 242.994 | -67.652 | 90.492 | 1.00 | 50.94 | A | . C |
| ATOM | 982 | CE1 | TYR . | A 246 | 244.042 | -67.382 | 89.609 | 1.00 | 55.86 | A | |
| ATOM | 983 | CD2 | TYR . | A 246 | 244.584 | -68.473 | 92.111 | | 54.39 | Z A | |
| ATOM | 984 | CE2 | | A 246 | | -68.213 | 91.234 | | 55.81 | A | |
| ATOM | 985 | CZ | | A 246 | | -67.665 | 89.982 | | 55.07 | | |
| ATOM | 986 | OH | | A 246 | | -67.409 | 89.112 | | 55.05 | | |
| ATOM | 987 | C | | A 246 | | -70.852 | 92.733 | | | | |
| | 988 | | | A 246 | | | | | 57.54 | <i>[</i> A | |
| ATOM | | 0 | | | | -71.322 | 91.718 | | 64.40 | Z A | |
| ATOM | 989 | N | | A 247 | | -71.180 | 93.951 | | 56.76 | P | |
| ATOM | 990 | CA | | A 247 | | -72.120 | 94.148 | | 57.81 | A | |
| MOTA | 991 | CB | | A 247 | | -72.066 | | 1.00 | 52.55 | ZA. | |
| ATOM | 992 | SG | | A 247 | 245.687 | -70.569 | 96.004 | 1.00 | 57.32 | 2 | . S |
| ATOM | 993 | C | CYS . | A 247 | 243.813 | -73.538 | 93.837 | 1.00 | 59.03 | 7 | , c |
| ATOM | 994 | 0 | CYS . | A 247 | 244.535 | -74.272 | 93.143 | 1.00 | 61.55 | A | |
| MOTA | 995 | N | HIS . | A 248 | 242.659 | -73.930 | 94.374 | | 60.08 | A | |
| ATOM | 996 | CA | HIS . | A 248 | 242.151 | -75.291 | 94.156 | | 58.63 | 7 | |
| ATOM | 997 | CB | | A 248 | | -75.540 | 95.036 | | 57.40 | ZA | |
| ATOM | 998 | CG | | A 248 | | -75.606 | | | 54.60 | .A | |
| ATOM | 999 | | | A 248 | | -75.694 | 97.160 | | 54.55 | | |
| ATOM | 1000 | | | A 248 | | -75.623 | | | | <i>7</i> 4 | |
| ATOM | | | | | | | 97.459 | | 54.23 | <i>P</i> . | |
| | 1001 | | | A 248 | | -75.721 | 98.654 | | 51.97 | A | |
| MOTA | 1002 | | | A 248 | | -75.765 | 98.501 | | 50.58 | A | |
| ATOM | 1003 | C | | A 248 | | -75.535 | 92.668 | | 58.67 | A | . C |
| ATOM | 1004 | 0 | | A 248 | | -76.667 | 92.171 | | 50.45 | A | . 0 |
| ATOM | 1005 | N | SER . | A 249 | 241.459 | -74.464 | 91.959 | | 53.97 | A | . N |
| MOTA | 1006 | CA | SER | A 249 | 241.133 | -74.589 | 90.550 | 1.00 | 58.32 | A | . C |
| ATOM | 1007 | CB | SER | A 249 | 240.647 | -73.248 | 89.991 | 1.00 | 55.40 | A | C |
| ATOM | 1008 | OG | SER | A 249 | 241.757 | -72.480 | 89.526 | 1.00 | 54.94 | A | . 0 |
| ATOM | 1009 | С | SER | A 249 | 242.407 | -75.020 | 89.798 | 1.00 | 58.15 | A | |
| MOTA | 1010 | 0 | SER | A 249 | 242.326 | -75.573 | 88.707 | | 70.94 | A | |
| ATOM | 1011 | N | | A 250 | | -74.746 | | | 51.49 | Z A | |
| ATOM | 1012 | CA | | A 250 | | -75.119 | 89.753 | | 46.67 | A | |
| MOTA | 1013 | CB | | A 250 | | -73.947 | 89.805 | | 31.37 | A | |
| ATOM | 1014 | c | | A 250 | | -76.343 | 90.494 | | 50.71 | A | |
| ATOM | 1015 | ŏ | | A 250 | | -76.755 | | | 60.01 | | |
| ATOM | 1016 | N | | A 251 | | -76.931 | 90.233 | | | A | |
| | | CA | | A 251 | | | | | 52.78 | A | |
| MOTA | 1017 | | | | | -78.113 | 92.167 | | 55.47 | A | _ |
| ATOM | 1018 | CB | | A 251 | | -79.258 | 91.244 | | 58.86 | A | _ |
| ATOM | 1019 | CG | | A 251 | | -79.957 | | | 62.01 | A | |
| ATOM | 1020 | CD | | A 251 | | -81.392 | 90.989 | 1.00 | 65.71 | A | . C |
| MOTA | 1021 | NE | | A 251 | | -81.741 | 91.512 | | 68.34 | A | . N |
| ATOM | 1022 | cz | | A 251 | | -82.945 | 92.002 | 1.00 | 72.31 | A | . С |
| ATOM | 1023 | | | A 251 | | -83.929 | 92.045 | 1.00 | 72.96 | A | . N |
| MOTA | 1024 | NH2 | ARG . | A 251 | 241.252 | -83.178 | 92.445 | 1.00 | 71.74 | A | . N |
| ATOM | 1025 | С | ARG . | A 251 | 246.099 | -77.840 | 93.137 | 1.00 | 53.93 | A | C |
| ATOM | 1026 | 0 | ARG . | A 251 | 247.007 | -78.666 | 93.285 | | 57.77 | A | |
| ATOM | 1027 | N | VAL . | A 252 | 246.043 | -76.686 | 93.799 | | 56.22 | A | |
| MOTA | 1028 | CA | | A 252 | | -76.314 | 94.774 | | 53.20 | A | |
| ATOM | 1029 | CB | | A 252 | | -74.966 | 94.401 | | 50.06 | A | |
| ATOM | 1030 | | | A 252 | | -74.549 | 95.463 | | 49.54 | | |
| ATOM | 1031 | | | A 252 | | -75.083 | 93.080 | | 48.46 | A | |
| MOTA | 1032 | C | | A 252 | | | | | | A | |
| | 1032 | | | | | -76.207 | 96.196 | | 54.67 | A | |
| ATOM | | 0 | | A 252 | | -75.465 -76.056 | 96.426 | | 56.55 | A | |
| ATOM | 1034 | N | | A 253 | | ~76.956 | 97.130 | | 52.34 | A | |
| ATOM | 1035 | CA | | A 253 | | -76.948 | 98.498 | | 42.71 | A | |
| ATOM | 1036 | CB | | A 253 | | -78.341 | 99.103 | | 38.24 | A | |
| ATOM | 1037 | | | A 253 | | -78.449 | | 1.00 | 44.12 | A | С |
| ATOM | 1038 | | | A 253 | | -79.380 | 98.083 | 1.00 | 35.92 | A | C |
| MOTA | 1039 | CD1 | ILE A | A 253 | 246.298 | -80.813 | 98.644 | | 42.55 | A | |
| ATOM | 1040 | С | ILE A | A 253 | 247.600 | -76.096 | 99.279 | | 48.08 | A | |
| ATOM | 1041 | 0 | | A 253 | | -76.288 | 99.163 | | 60.87 | A | |
| ATOM | 1042 | N | | A 254 | | -75.165 | | | 50.60 | A | |
| | | | | _ = • | | | | | 55.55 | n | TA |

| ATOM | 1043 | CA | HIS | Α | 254 | 247.955 | -74.319 | 100.906 | 1.00 | 45.11 | A | . с |
|------|------|------|-----|---|-----|---------|---------|---------|------|-------|----------|-----|
| ATOM | 1044 | CB | HIS | Δ | 254 | | -73.086 | | | 43.92 | A | . с |
| | | CG | | | | _ | | _ | | | | |
| MOTA | 1045 | | HIS | | | | -72.014 | | | 44.85 | A | |
| MOTA | 1046 | CD2 | HIS | А | 254 | 248.486 | -70.854 | 101.360 | 1.00 | 39.20 | A | . C |
| ATOM | 1047 | ND1 | HIS | Α | 254 | 248.670 | -72.089 | 103.158 | 1.00 | 39.59 | A | N |
| ATOM | 1048 | CE1 | HIS | Δ | 254 | | -71.014 | | | 37.61 | A | |
| | | | | | | | | | | | | |
| MOTA | 1049 | | HIS | | | | -70.250 | | 1.00 | 38.54 | A | |
| MOTA | 1050 | С | HIS | Α | 254 | 248.490 | -75.117 | 102.103 | 1.00 | 44.15 | P | C |
| ATOM | 1051 | 0 | HIS | А | 254 | 249.681 | -75.123 | 102.372 | 1.00 | 48.22 | P | . 0 |
| | | N | ARG | | | | -75.802 | | | | | |
| MOTA | 1052 | | | | | | | | | 42.94 | A | |
| MOTA | 1053 | CA | ARG | Α | 255 | 247.899 | -76.642 | 103.946 | 1.00 | 38.93 | A | C |
| MOTA | 1054 | CB | ARG | Α | 255 | 248.829 | ~77.796 | 103.512 | 1.00 | 44.03 | A | C |
| MOTA | 1055 | CG | ARG | Δ | 255 | 248.460 | -78.369 | 102 124 | 1 00 | 46.01 | P | C |
| | | | | | | | -79.689 | | | | | |
| ATOM | 1056 | CD | ARG | | | | | | | 54.38 | A | |
| MOTA | 1057 | NE | ARG | A | 255 | 250.581 | -79.648 | 102.175 | 1.00 | 53.55 | A | N |
| ATOM | 1058 | CZ | ARG | Α | 255 | 251.402 | -80.673 | 102.012 | 1.00 | 53.89 | P | L C |
| ATOM | 1059 | NH1 | ARG | А | 255 | 250.938 | -81.808 | 101.562 | 1.00 | 52.04 | P | N |
| | | | | | | | -80.560 | | | | | |
| MOTA | 1060 | | ARG | | | | | | | 55.38 | P | |
| MOTA | 1061 | С | ARG | Α | 255 | 248.477 | -75.929 | 105.145 | 1.00 | 37.93 | P | C |
| ATOM | 1062 | 0 | ARG | Α | 255 | 248.891 | -76.588 | 106.101 | 1.00 | 37.60 | P | 0 |
| MOTA | 1063 | N | ASP | Δ | 256 | 248.541 | -74.598 | 105.096 | 1.00 | 40.81 | P | N |
| | | | | | 256 | | -73.852 | | | | | |
| ATOM | 1064 | CA | | | | | | | | 41.86 | P | |
| MOTA | 1065 | CB | ASP | A | 256 | | -73.685 | | 1.00 | 38.62 | P | C C |
| ATOM | 1066 | CG | ASP | A | 256 | 251.299 | -73.245 | 107.284 | 1.00 | 42.25 | P | v C |
| MOTA | 1067 | OD1 | ASP | А | 256 | 250.822 | -73.586 | 108.373 | | 44.21 | P | . 0 |
| | | | ASP | | | | -72.594 | | | 39.16 | | |
| MOTA | 1068 | | | | | | | | | | P | |
| MOTA | 1069 | С | ASP | Α | 256 | | -72.491 | | 1.00 | 45.37 | P | v C |
| ATOM | 1070 | 0 | ASP | Α | 256 | 249.065 | -71.464 | 106.563 | 1.00 | 52.63 | F | . 0 |
| ATOM | 1071 | N | TIF | А | 257 | 247.092 | -72.503 | 106.340 | 1.00 | 49.04 | P | N A |
| | 1072 | CA | | | 257 | | -71.289 | | | 56.39 | F | |
| MOTA | | | | | | | | | | - | | |
| MOTA | 1073 | CB | ILE | Α | 257 | 244.939 | -71.461 | 105.776 | 1.00 | 52.32 | F | A C |
| ATOM | 1074 | CG2 | ILE | Α | 257 | 244.163 | -70.205 | 105.893 | 1.00 | 55.85 | P | Y C |
| ATOM | 1075 | CG1 | ILE | А | 257 | 245.143 | -71.785 | 104.305 | 1.00 | 60.94 | P | . C |
| | 1076 | | ILE | | | | -72.064 | | | 73.36 | 7 | |
| MOTA | | | | | | | | | | | | |
| ATOM | 1077 | С | | | 257 | | -70.940 | | 1.00 | 54.79 | P | A C |
| ATOM | 1078 | 0 | ILE | Α | 257 | 245.502 | -71.720 | 108.659 | 1.00 | 61.06 | F | . 0 |
| MOTA | 1079 | N | LYS | Α | 258 | 246.594 | -69.781 | 108.345 | 1.00 | 50.33 | F | A N |
| MOTA | 1080 | CA | | | 258 | | -69.356 | | | 46.70 | | C |
| | | | | | | | | | | | | |
| ATOM | 1081 | CB | | | 258 | | -70.220 | | | 41.61 | | A C |
| MOTA | 1082 | CG | LYS | Α | 258 | 248.687 | -70.371 | 110.232 | 1.00 | 49.22 | F | A C |
| MOTA | 1083 | CD | LYS | Α | 258 | 249.425 | -71.326 | 111,200 | 1.00 | 42.38 | F | A C |
| MOTA | 1084 | CE | | | 258 | | -71.627 | | | 51.66 | | A C |
| | | | | | | | | | | | | |
| MOTA | 1085 | ΝZ | | | 258 | | -72.718 | | | 40.89 | F | |
| ATOM | 1086 | С | LYS | Α | 258 | 246.756 | -67.876 | 109.860 | 1.00 | 45.25 | F | A C |
| MOTA | 1087 | 0 | LYS | Α | 258 | 247.504 | -67.337 | 109.042 | 1.00 | 41.75 | F | A 0 |
| ATOM | 1088 | N | PRO | Δ | 259 | 246.189 | -67.209 | 110 898 | 1.00 | 38.54 | F | A N |
| | 1089 | - | | | 259 | | -67.848 | | | | | |
| MOTA | | CD | | | | | | | | 30.99 | | C |
| ATOM | 1090 | CA | | | 259 | | -65.786 | | | 33.18 | F | A C |
| MOTA | 1091 | CB | PRO | Α | 259 | 246.034 | -65.680 | 112.643 | 1.00 | 36.45 | F | A C |
| ATOM | 1092 | CG | PRO | Α | 259 | 244.915 | -66.649 | 112.762 | 1.00 | 29.46 | F | A C |
| ATOM | 1093 | С | PRO | Δ | 259 | | -65.250 | | | 39.75 | F | |
| | | | | | | | | | | | | |
| MOTA | 1094 | 0 | | | 259 | | -64.163 | | | 46.84 | F | |
| ATOM | 1095 | N | | | 260 | 248.836 | ~65.999 | 111.177 | 1.00 | 43.95 | F | A N |
| ATOM | 1096 | CA | GLU | Α | 260 | 250.227 | -65.591 | 110.916 | 1.00 | 44.86 | F | 7 C |
| MOTA | 1097 | CB | | | 260 | | -66.603 | | | 50.78 | F | |
| | | | | | | | -66.922 | | | | | |
| MOTA | 1098 | CG | | | 260 | | | | | 65.67 | F | |
| ATOM | 1099 | CD | | | 260 | 249.918 | -67.897 | 113.213 | 1.00 | 69.34 | F | A C |
| ATOM | 1100 | OE1 | GLU | Α | 260 | 248.727 | -67.499 | 113.338 | 1.00 | 69.34 | P | . 0 |
| ATOM | 1101 | OE 2 | GLU | Δ | 260 | 250.264 | -69.089 | 113.299 | 1 00 | 80.21 | P | |
| | | | | | | | -65.476 | | | | | |
| MOTA | 1102 | С | | | 260 | | | | | 39.11 | F | |
| ATOM | 1103 | 0 | | | 260 | | -64.554 | | 1.00 | 44.76 | P | 7 0 |
| ATOM | 1104 | N | ASN | Α | 261 | 250.029 | -66.425 | 108.622 | 1.00 | 40.15 | P | N |
| ATOM | 1105 | CA | | | 261 | | -66.396 | | | 38.92 | P | |
| | | | | | | | -67.817 | | | | | |
| MOTA | 1106 | CB | | | 261 | | | | | 36.39 | P | |
| ATOM | 1107 | CG | | | 261 | | -68.579 | | | 36.54 | P | |
| ATOM | 1108 | OD1 | ASN | A | 261 | 252.609 | -68.045 | 107.462 | 1.00 | 41.73 | P | . 0 |
| MOTA | 1109 | צמא | ASN | Α | 261 | 251.317 | -69.831 | 107.578 | | 30.81 | A | N |
| | 1110 | C | | | 261 | | | 106.361 | | 38.95 | P | |
| MOTA | | | | | | | | | | | | |
| MOTA | 1111 | 0 | | | 261 | | | 105.149 | | 40.40 | P | |
| MOTA | 1112 | N | LEU | Α | 262 | 248.245 | -64.953 | 107.046 | 1.00 | 42.51 | A | N |
| | | | | | | | | | | | | |

| ATOM | 1113 | CA | LEU | Δ | 262 | 247.197 -64.169 106.386 1.00 42.29 | | _ |
|------|------|------|------|-----|-----|------------------------------------|----|---|
| ATOM | 1114 | CB | | | 262 | | A | C |
| | | | | | | 245.800 -64.450 106.967 1.00 36.57 | A | C |
| MOTA | 1115 | CG | | | 262 | 245.209 -65.819 106.657 1.00 37.41 | A | С |
| MOTA | 1116 | | | | 262 | 243.773 -65.817 107.071 1.00 33.79 | A | С |
| MOTA | 1117 | CD2 | LEU | Α | 262 | 245.324 -66.152 105.193 1.00 39.29 | A | C |
| ATOM | 1118 | С | LEU | Α | 262 | 247.548 -62.703 106.582 1.00 41.70 | A | Č |
| MOTA | 1119 | O | | | 262 | 0.4m m.s | | |
| | 1120 | | | | | | A | 0 |
| ATOM | | N_ | | | 263 | 247.857 -62.021 105.473 1.00 38.70 | A | N |
| MOTA | 1121 | CA | | | 263 | 248.238 -60.610 105.505 1.00 26.99 | A | С |
| ATOM | 1122 | CB | LEU | A | 263 | 249.475 -60.392 104.679 1.00 36.05 | A | С |
| MOTA | 1123 | CG | LEU | A | 263 | 250.658 -61.333 104.917 1.00 31.41 | A | C |
| ATOM | 1124 | CD1 | | | 263 | 251.820 -60.991 103.978 1.00 33.22 | | |
| ATOM | 1125 | | | | 263 | | A | C |
| | | | | | | 251.081 -61.269 106.325 1.00 29.25 | A | С |
| MOTA | 1126 | С | | | 263 | 247.144 -59.677 105.013 1.00 35.80 | A | С |
| MOTA | 1127 | 0 | | | 263 | 246.220 -60.100 104.304 1.00 32.87 | A | 0 |
| MOTA | 1128 | N | LEU | Α | 264 | 247.245 -58.408 105.410 1.00 31.98 | A | N |
| ATOM | 1129 | CA | LEU | Α | 264 | 246.246 -57.428 105.041 1.00 33.35 | A | C |
| ATOM | 1130 | СВ | | | 264 | | | |
| | 1131 | CG | | | 264 | | A | C |
| ATOM | | | | | | 244.971 -57.619 107.303 1.00 28.92 | A | C |
| ATOM | 1132 | | | | 264 | 244.728 -56.820 108.620 1.00 24.69 | A | С |
| ATOM | 1133 | CD2 | LEU | A | 264 | 243.644 -58.095 106.660 1.00 26.84 | A | С |
| MOTA | 1134 | С | LEU | A | 264 | 246.884 ~56.419 104.110 1.00 35.86 | A | С |
| ATOM | 1135 | 0 | LEU | A | 264 | 247.974 -55.944 104.368 1.00 40.12 | A | ŏ |
| ATOM | 1136 | N | | | 265 | | | |
| | | | | | | 246.188 -56.100 103.026 1.00 36.89 | A | N |
| ATOM | 1137 | CA | | | 265 | 246.674 -55.133 102.045 1.00 43.31 | A | С |
| MOTA | 1138 | С | GLY | Α | 265 | 246.399 -53.673 102.351 1.00 43.89 | A | C |
| ATOM | 1139 | 0 | GLY | Α | 265 | 245.889 -53.350 103.401 1.00 48.54 | A | 0 |
| ATOM | 1140 | N | SER | A | 266 | 246.742 -52.796 101.422 1.00 48.23 | A | N |
| ATOM | 1141 | CA | | | 266 | 246.567 -51.364 101.591 1.00 49.09 | | |
| ATOM | 1142 | CB | | | 266 | | A | C |
| | | | | | | 246.936 -50.647 100.304 1.00 51.41 | A | C |
| ATOM | 1143 | OG | | | 266 | 246.057 -51.012 99.237 1.00 64.31 | A. | 0 |
| ATOM | 1144 | С | SER | A | 266 | 245.138 -51.019 101.970 1.00 51.39 | A | С |
| MOTA | 1145 | 0 | SER | A | 266 | 244.915 -50.247 102.883 1.00 54.83 | A | 0 |
| ATOM | 1146 | N | ALA | A | 267 | 244.162 -51.588 101.271 1.00 54.20 | A | N |
| ATOM | 1147 | CA | | | 267 | A.A | | |
| ATOM | 1148 | CB | | | 267 | | A | C |
| | | | | | | 241.921 -51.394 100.320 1.00 47.18 | Α | С |
| MOTA | 1149 | C | | | 267 | 242.203 -52.330 102.595 1.00 48.50 | A. | С |
| ATOM | 1150 | 0 | ALA | . A | 267 | 241.010 -52.582 102.620 1.00 50.25 | A | 0 |
| ATOM | 1151 | N | GLY | Α | 268 | 243.084 -52.913 103.410 1.00 45.91 | A | N |
| ATOM | 1152 | CA | GLY | Α | 268 | 242.665 -53.860 104.420 1.00 38.28 | A | C |
| ATOM | 1153 | С | GT.Y | Δ | 268 | 242.192 -55.187 103.868 1.00 42.82 | | č |
| ATOM | 1154 | ō | | | 268 | | A | |
| | | | | | | | A | 0 |
| ATOM | 1155 | N | | | 269 | 242.396 -55.431 102.569 1.00 42.29 | A | И |
| ATOM | 1156 | CA | | | 269 | 241.958 -56.697 101.992 1.00 40.12 | A | C |
| ATOM | 1157 | CB | GLU | A | 269 | 241.996 -56.635 100.480 1.00 44.93 | A | С |
| ATOM | 1158 | ÇG | GLU | Α | 269 | 243.430 -56.655 99.871 1.00 51.34 | A | C |
| ATOM | 1159 | CĐ | GLU | Α | 269 | 243.997 -55.261 99.657 1.00 57.16 | A | č |
| ATOM | 1160 | OE 1 | GT.U | Δ | 269 | 244.081 -54.491 100.642 1.00 51.07 | | |
| ATOM | 1161 | | | | 269 | | A | 0 |
| | | | | | | 244.350 -54.945 98.493 1.00 61.02 | A | 0 |
| ATOM | 1162 | C. | | | 269 | 242.872 -57.847 102.472 1.00 44.10 | A | С |
| ATOM | 1163 | 0 | GLU | A | 269 | 244.053 -57.652 102.807 1.00 43.32 | A | 0 |
| MOTA | 1164 | N | LEU | Α | 270 | 242.331 -59.059 102.481 1.00 43.44 | A | N |
| ATOM | 1165 | CA | LEU | Α | 270 | 243.076 -60.228 102.927 1.00 44.15 | A | Ċ |
| ATOM | 1166 | СВ | | | 270 | 242.102 -61.333 103.323 1.00 50.71 | | |
| ATOM | 1167 | CG | | | 270 | | A | C |
| | | | | | | | A | С |
| ATOM | 1168 | | | | 270 | 242.304 -62.033 105.661 1.00 60.78 | A | С |
| ATOM | 1169 | CD2 | | | 270 | 241.999 -63.736 103.906 1.00 50.44 | A | C |
| ATOM | 1170 | С | LEU | Α | 270 | 243.985 -60.731 101.813 1.00 44.35 | A | С |
| MOTA | 1171 | 0 | LEU | A | 270 | 243.728 -60.526 100.635 1.00 49.43 | A | ō |
| ATOM | 1172 | N | | | 271 | 245.063 -61.398 102.188 1.00 40.19 | | |
| ATOM | 1173 | CA | | | 271 | | A | И |
| | | | | | | | A | С |
| ATOM | 1174 | CB | | | 271 | 247.028 -60.897 100.819 1.00 32.47 | A | С |
| MOTA | 1175 | CG | | | 271 | 246.604 -59.930 99.753 1.00 31.86 | Α | C |
| ATOM | 1176 | CD | LYS | A | 271 | 247.492 -58.692 99.731 1.00 35.87 | A | Č |
| ATOM | 1177 | CE | LYS | Α | 271 | 247.103 -57.715 98.619 1.00 42.09 | A | c |
| ATOM | 1178 | NZ | | | 271 | 247.551 -58.225 97.303 1.00 58.37 | A | |
| ATOM | 1179 | C | | | 271 | | | N |
| | | | | | | | A | С |
| ATOM | 1180 | 0 | | | 271 | 247.433 -63.023 102.807 1.00 49.74 | A | 0 |
| ATOM | 1181 | N | | | 272 | 246.505 -64.322 101.249 1.00 39.27 | Α | N |
| MOTA | 1182 | CA | ILE | Α | 272 | 247.155 -65.524 101.741 1.00 34.76 | A | C |
| | | | | | | | | - |

| ATOM | 1183 | CB | ILE | A | 272 | 246.491 | -66.758 | 101.150 | 1.00 | 44.34 | | Α | С |
|------|------|-----|-----|---|-----|---------|---------|---------|------|-------|---|----|---|
| ATOM | 1184 | | ILE | | | 246.821 | -67.987 | 102.002 | 1.00 | 55.36 | | A | С |
| MOTA | 1185 | CG1 | ILE | Α | 272 | 244.973 | -66.577 | 101.161 | | 50.03 | | A | С |
| MOTA | 1186 | | ILE | | | | -67.794 | | | 52.97 | | A | Č |
| ATOM | 1187 | C | | | 272 | | -65.530 | | | 41.49 | | A | č |
| ATOM | 1188 | ō | | | 272 | | -65.272 | | | 40.02 | | A | ŏ |
| ATOM | 1189 | N | | | 273 | | -65.832 | | | 39.46 | | | |
| MOTA | 1190 | CA | | | | | | | | | | A | N |
| | | | | | 273 | | -65.861 | | | 38.71 | | A | C |
| ATOM | 1191 | CB | | | 273 | | -64.617 | | | 40.33 | | A | С |
| ATOM | 1192 | C . | | • | 273 | | -67.137 | | | 46.92 | | A | С |
| ATOM | 1193 | 0 | | | 273 | | -68.063 | | 1.00 | 49.16 | | A | 0 |
| MOTA | 1194 | N | ASP | A | 274 | | -67.165 | | 1.00 | 51.43 | | A | N |
| ATOM | 1195 | CA | ASP | Α | 274 | 253.703 | -68.293 | 102.997 | 1.00 | 51.40 | | A | С |
| ATOM | 1196 | CB | ASP | Α | 274 | 253.686 | -68.323 | 104.530 | 1.00 | 50.98 | | A | С |
| ATOM | 1197 | CG | ASP | Α | 274 | 254.601 | -69.361 | 105.083 | 1.00 | 42.10 | | A | C |
| MOTA | 1198 | OD1 | ASP | Α | 274 | 255.660 | -69.637 | 104.516 | 1.00 | 54.26 | | A | 0 |
| MOTA | 1199 | OD2 | ASP | Α | 274 | | -69.914 | | | 52.11 | | A | ō |
| ATOM | 1200 | С | | | 274 | | -69.618 | | | 51.38 | | A | Č |
| MOTA | 1201 | 0 | | | 274 | | -70.382 | | | 53.85 | | A | ő |
| ATOM | 1202 | N | | | 275 | | -69.863 | | | 53.60 | | A | N |
| ATOM | 1203 | CA | | | 275 | | ~71.097 | | | | | | |
| ATOM | 1203 | CB | | | 275 | | | | | 46.97 | | A | C |
| | 1204 | | | | | | -70.871 | 98.973 | | 42.90 | | A | C |
| MOTA | | CG | | | 275 | | -70.169 | 98.636 | | 45.54 | | A | С |
| ATOM | 1206 | | PHE | | | | -68.830 | | | 45.75 | | A | С |
| MOTA | 1207 | | PHE | | | | -70.843 | | | 41.77 | | A | С |
| ATOM | 1208 | | PHE | | | 250.305 | -68.152 | 98.737 | 1.00 | 48.01 | | A | С |
| MOTA | 1209 | CE2 | PHE | A | 275 | | -70.195 | 97.591 | 1.00 | 46.76 | | A | С |
| ATOM | 1210 | CZ | PHE | Α | 275 | | -68.840 | 98.000 | 1.00 | 48.77 | | A | С |
| ATOM | 1211 | С | PHE | Α | 275 | 254.270 | -72.149 | 100.678 | 1.00 | 43.41 | | A | С |
| ATOM | 1212 | 0 | PHE | Α | 275 | 254.496 | -72.970 | 99.791 | 1.00 | 36.81 | | A | 0 |
| MOTA | 1213 | N | GLY | Α | 276 | 254.938 | -72.109 | 101.843 | | 42.93 | | A | N |
| ATOM | 1214 | CA | GLY | Α | 276 | | -73.079 | | | 37.83 | | A | c |
| ATOM | 1215 | С | GLY | Α | 276 | | -74.522 | | | 35.71 | | A | Č |
| MOTA | 1216 | 0 | | | 276 | | -75.412 | | | 45.98 | | A | ŏ |
| ATOM | 1217 | Ŋ | | | 277 | | -74.768 | | | 40.57 | | A | N |
| ATOM | 1218 | CA | | | 277 | | -76.118 | | | 36.62 | | A | C |
| ATOM | 1219 | CB | | | 277 | | -76.378 | | | | | | |
| MOTA | 1220 | CG | | | 277 | | -76.592 | | | 42.09 | | A | C |
| ATOM | 1221 | | TRP | | | | -77.854 | | | 50.97 | | A | C |
| | 1222 | | | | | | | | | 58.62 | | A | C |
| MOTA | | | TRP | | | | -77.593 | | | 58.91 | | A | С |
| MOTA | 1223 | | TRP | | | | -79.182 | | | 59.93 | | A | C |
| ATOM | 1224 | | TRP | | | | -75.640 | | | 54.30 | | A | C |
| ATOM | 1225 | | TRP | | | | -76.235 | | | 59.86 | | A | N |
| ATOM | 1226 | | TRP | | | | -78.610 | | | 61.19 | | A | C |
| MOTA | 1227 | | TRP | | | 254.244 | -80.188 | 106.162 | 1.00 | 61.29 | | A | C |
| ATOM | 1228 | CH2 | TRP | | | | -79.892 | | 1.00 | 63.73 | | A | C |
| MOTA | 1229 | С | TRP | Α | 277 | 252.777 | -76.364 | 101.408 | 1.00 | 35.74 | | A | С |
| MOTA | 1230 | 0 | | | 277 | 252.212 | -77.442 | 101.298 | 1.00 | 35.61 | | A | 0 |
| MOTA | 1231 | N | SER | Α | 278 | 252.636 | -75.372 | 100.528 | 1.00 | 44.94 | | A. | N |
| ATOM | 1232 | CA | SER | Α | 278 | 251.779 | -75.474 | 99.336 | 1.00 | 46.77 | | A | С |
| ATOM | 1233 | CB | SER | A | 278 | 251.916 | -74.202 | 98.517 | 1.00 | 42.80 | | A. | С |
| ATOM | 1234 | OG | SER | Α | 278 | 250.880 | -74.139 | 97.565 | 1.00 | 54.88 | | A | ō |
| ATOM | 1235 | С | SER | Α | 278 | 252.200 | -76.703 | 98.464 | | 50.47 | | A | Č |
| ATOM | 1236 | 0 | SER | Α | 278 | | -77.084 | 98.378 | | 54.17 | | A | ŏ |
| ATOM | 1237 | N | VAL | | | | -77.347 | 97.819 | | 51.50 | | A | N |
| ATOM | 1238 | CA | VAL | | | | -78.514 | 96.992 | | 57.94 | | A | C |
| ATOM | 1239 | СВ | VAL | | | | -79.780 | 97.847 | | 44.98 | | | |
| ATOM | 1240 | | VAL | | | 250.199 | | 97.997 | | 43.31 | | A. | C |
| ATOM | 1241 | | VAL | | | 252.491 | | 97.178 | | | | A | C |
| | 1242 | | | | | | | | | 57.04 | | A. | C |
| MOTA | | C | VAL | | | 250.626 | | 95.765 | | 59.15 | | A. | C |
| ATOM | 1243 | 0 | VAL | | | 249.430 | | 95.867 | | 67.05 | | A. | 0 |
| ATOM | 1244 | N | HIS | | | 251.204 | | 94.615 | | 63.81 | | A. | N |
| ATOM | 1245 | CA | HIS | | | 250.486 | | 93.335 | | 67.43 | | A | С |
| MOTA | 1246 | CB | HIS | | | 251.439 | | 92.122 | | 66.79 | 1 | A, | С |
| ATOM | 1247 | CG | HIS | | | 250.875 | | 91.056 | 1.00 | 72.05 | | A | С |
| ATOM | 1248 | | HIS | | | 250.729 | | 89.721 | 1.00 | 75.11 | i | Ą | С |
| MOTA | 1249 | | HIS | | | 250.404 | -76.921 | 91.326 | 1.00 | 73.34 | i | A | N |
| ATOM | 1250 | CE1 | HIS | А | 280 | 249.997 | -76.358 | 90.201 | | 80.03 | | Ą | С |
| ATOM | 1251 | NE2 | HIS | A | 280 | 250.185 | -77.217 | 89.213 | | 83.14 | | A | N |
| ATOM | 1252 | С | HIS | А | 280 | 249.968 | -80.672 | 93.390 | | 70.50 | | 4 | C |
| | | | | | | | | | | | - | | - |

| ATOM | 1253 | 0 | HIS | A | 280 | | -81.589 | 92.745 | 1.00 82.51 | A | 0 |
|--------------|--------------|----------|------------|----|------------|---------|--------------------|------------------|--------------------------|--------|--------|
| MOTA | 1254 | N | ALA | | | | -80.853 | 93.985 | 1.00 68.02 | A | N |
| ATOM | 1255 | CA | ALA | | | | -82.260 | 94.196 | 1.00 68.33 | A | С |
| MOTA | 1256 | CB C | ALA | | | | -82.885 | 94.806 | 1.00 60.98 | A | C |
| MOTA MOTA | 1257 1258 | 0 | ALA | | | | -82.754 -82.032 | 95.016 95.339 | 1.00 68.64 1.00 67.99 | A n | C |
| ATOM | 1259 | N | | | 282 | | -84.034 | 95.373 | 1.00 70.43 | A A | И |
| MOTA | 1260 | CD | | | 282 | | -84.236 | 93.943 | 1.00 64.78 | A | Č |
| ATOM | 1261 | CA | | | 282 | | -85.171 | 96.058 | 1.00 67.06 | A | Ċ |
| MOTA | 1262 | CB | PRO | Α | 282 | 246.654 | -86.295 | 95.053 | 1.00 67.65 | A | С |
| MOTA | 1263 | CG | | | 282 | | -85.826 | 93.934 | 1.00 63.34 | A | С |
| ATOM | 1264 | C | | | 282 | | -85.384 | 96.902 | 1.00 69.62 | A | С |
| MOTA | 1265 | O N | | | 282 283 | | -85.628 | 96.346 | 1.00 80.00 | A | 0 |
| MOTA MOTA | 1266 1267 | CA | | | 283 | | -85.322 -85.680 | 98.204 98.758 | 1.00 65.02 1.00 59.53 | A A | N C |
| ATOM | 1268 | CB | | | 283 | | -84.498 | 98.799 | 1.00 55.46 | A | Č |
| ATOM | 1269 | OG | | | 283 | | -84.456 | | 1.00 55.84 | A | ō |
| ATOM | 1270 | С | SER | A | 283 | | -86.394 | | 1.00 55.99 | A | С |
| MOTA | 1271 | 0 | | | 283 | | -86.609 | | 1.00 69.93 | A | 0 |
| ATOM | 1272 | N | | | 284 | | -86.835 | | 1.00 60.56 | A | N |
| MOTA | 1273 | CA | | | 284 | | -87.467 | | 1.00 63.49 | A | C |
| ATOM ATOM | 1274 1275 | CB OG | | | 284 284 | | -88.808 -88.697 | | 1.00 63.76 1.00 77.24 | A | C |
| ATOM | 1276 | C | | | 284 | | -86.432 | | 1.00 77.24 | A A | 0 |
| ATOM | 1277 | Õ | | | 284 | | -85.336 | | 1.00 57.98 | A | ő |
| MOTA | 1278 | N | | | 285 | | -86.775 | | 1.00 64.16 | A | N |
| MOTA | 1279 | CA | | | 285 | • | -85.889 | | 1.00 67.66 | A | С |
| ATOM | 1280 | CB | | | 285 | | -86.301 | | 1.00 62.91 | A | С |
| ATOM | 1281 | С | | | 285 | | -85.923 | | 1.00 68.61 | A | C |
| ATOM ATOM | 1282 1283 | И О | | | 285 286 | | -86.645 -85.146 | | 1.00 72.84 1.00 71.24 | A | O N |
| ATOM | 1284 | CA | | | 286 | | -85.059 | | 1.00 71.24 | A A | C |
| ATOM | 1285 | СВ | | | 286 | | -83.563 | | 1.00 73.44 | A | č |
| MOTA | 1286 | CG | ARG | A | 286 | | -82.698 | | 1.00 71.75 | A | C |
| MOTA | 1287 | CD | | | 286 | | -83.449 | | 1.00 72.37 | A | C |
| MOTA | 1288 | NE | | | 286 | | -82.999 | | 1.00 72.92 | A | N |
| ATOM ATOM | 1289 1290 | CZ | ARG | | 286 | | -83.207 -83.858 | 99.989 | 1.00 77.01 | A | C |
| ATOM | 1291 | | ARG | | | | -82.753 | 98.778 | 1.00 80.80 1.00 73.00 | A A | N N |
| ATOM | 1292 | C | | | 286 | | -85.649 | | 1.00 79.18 | A | C |
| MOTA | 1293 | 0 | ARG | Α | 286 | | -85.258 | | 1.00 80.60 | A | Õ |
| MOTA | 1294 | N | | | 287 | 256.458 | -86.471 | 106.097 | 1.00 82.59 | A | N |
| ATOM | 1295 | CA | | | 287 | | -87.091 | | 1.00 81.36 | A | С |
| ATOM | 1296 | CB | TPO | | 287 | | -87.583 | | 1.00 85.77 | A | C |
| ATOM ATOM | 1297 1298 | OG1 | | | 287 | | -88.436 -87.965 | | 1.00 78.62 1.00 96.25 | A | C |
| ATOM | 1299 | P | | | 287 | | -89.537 | | 1.00 94.25 | A A | P |
| MOTA | 1300 | | TPO | | | | -89.889 | | 1.00105.80 | A | ō |
| MOTA | 1301 | | TPO | | | 259.793 | -89.485 | 104.142 | 1.00103.14 | A | 0 |
| MOTA | 1302 | | TPO | | | | -90.552 | | 1.00103.19 | A | 0 |
| MOTA | 1303 | C | | | 287 | | -86.093 | | 1.00 84.40 | A | С |
| ATOM ATOM | 1304 1305 | N N | | | 287 288 | | -86.453 -84.776 | | 1.00 82.15 | A | 0 |
| ATOM | 1305 | CA | | | 288 | | -84.113 | | 1.00 86.52 1.00 85.55 | A A | N C |
| ATOM | 1307 | CB | | | 288 | | -83.387 | | 1.00 87.59 | A | c |
| MOTA | 1308 | | TPO | | | | -83.063 | | 1.00 82.26 | A | Ċ |
| ATOM | 1309 | OG1 | TPO | | | | -83.759 | | 1.00 93.55 | A | 0 |
| ATOM | 1310 | P | | | 288 | | -84.822 | | 1.00 87.77 | A | ₽ |
| MOTA | 1311 | | TPO | | | | -83.892 | | 1.00 91.79 | A | 0 |
| ATOM ATOM | 1312 1313 | | TPO TPO | | | | -85.656 -85.456 | | 1.00 93.35 | A | 0 |
| ATOM | 1313 | C | TPO | | | | -82.985 | | 1.00 95.16 1.00 89.28 | A A | 0 |
| MOTA | 1315 | Ö | | | 288 | | -82.594 | | 1.00 86.14 | A | õ |
| ATOM | 1316 | N | | | 289 | 256.536 | -82.411 | 111.055 | 1.00 87.01 | A | N |
| ATOM | 1317 | CA | | | 289 | | -81.523 | | 1.00 88.25 | A | С |
| ATOM | 1318 | CB | | | 289 | | -82.345 | | 1.00 78.91 | A | C |
| ATOM | 1319 | C | LEU | | | | -80.565 | | 1.00 87.34 | A | С |
| ATOM ATOM | 1320 1321 | N O | LEU CYS | | | | -80.894 -79.389 | | 1.00 90.27 1.00 89.51 | A | O |
| ATOM | 1322 | CA | CYS | | | | -78.354 | | 1.00 89.51 | A A | С |
| 01-1 | | 023 | 010 | -1 | 200 | 200.047 | ,0.554 | | x.00 03.13 | • | C |

| MOTA | 1323 | СВ | CYS A 290 | 257.299 -77.405 112.324 1.00 80.05 | A | С |
|--------------|--------------|-----------|----------------------------|--|--------|--------|
| MOTA | 1324 | С | CYS A 290 | 254.931 -77.891 112.490 1.00 90.22 | A | Ċ |
| MOTA | 1325 | 0 | CYS A 290 | 254.405 -77.933 111.292 1.00 91.11 | A | 0 |
| ATOM | 1326 | N | GLY A 291 | 254.262 -77.496 113.541 1.00 90.88 | Α | N |
| MOTA | 1327 | CA | GLY A 291 | 252.946 -77.026 113.294 1.00 84.36 | Α | С |
| MOTA | 1328 | С | GLY A 291 | 252.214 -77.175 114.559 1.00 80.67 | A | С |
| ATOM | 1329 | 0 | GLY A 291 | 252.395 -78.093 115.381 1.00 72.19 | A | 0 |
| MOTA | 1330 | N | THR A 292 | 251.411 -76.152 114.668 1.00 72.87 | Α | N |
| ATOM | 1331 | CA | THR A 292 | 250.543 -75.923 115.732 1.00 68.66 | A | С |
| MOTA | 1332 | CB | THR A 292 | 250.229 -74.450 115.788 1.00 64.26 | A | С |
| MOTA | 1333 1334 | | L THR A 292 2 THR A 292 | | A | 0 |
| MOTA MOTA | 1335 | C | THR A 292 | | A | C |
| ATOM | 1336 | ō | THR A 292 | 249.401 -76.698 115.093 1.00 69.67 248.736 -76.230 114.162 1.00 81.32 | A | C |
| ATOM | 1337 | N | LEU A 293 | 248.736 -76.230 114.162 1.00 81.32 249.162 -77.905 115.545 1.00 65.76 | A | 0 |
| MOTA | 1338 | CA | LEU A 293 | 248.076 -78.633 114.929 1.00 57.85 | A A | N C |
| ATOM | 1339 | СВ | LEU A 293 | 247.775 -79.863 115.741 1.00 58.26 | A | C |
| ATOM | 1340 | CG | LEU A 293 | 249.007 -80.649 116.175 1.00 59.75 | A | č |
| ATOM | 1341 | CD1 | LEU A 293 | 248.607 -81.606 117.246 1.00 56.85 | A | c |
| MOTA | 1342 | CD2 | LEU A 293 | 249.618 -81.397 114.982 1.00 55.33 | A | Ċ |
| MOTA | 1343 | С | LEU A 293 | 246.812 -77.819 114.737 1.00 54.37 | A | C |
| ATOM | 1344 | 0 | LEU A 293 | 246.215 -77.930 113.686 1.00 59.11 | A | 0 |
| ATOM | 1345 | N | ASP A 294 | 246.467 -76.947 115.687 1.00 45.72 | Α | N |
| ATOM | 1346 | CA | ASP A 294 | 245.241 -76.166 115.622 1.00 46.04 | Α | С |
| ATOM | 1347 | CB | ASP A 294 | 245.471 -74.762 116.195 1.00 47.18 | A | С |
| ATOM | 1348 | CG | ASP A 294 | 245.754 -74.782 117.713 1.00 53.87 | A | C |
| MOTA MOTA | 1349 1350 | | ASP A 294 ASP A 294 | 244.938 -75.399 118.452 1.00 53.07 | A | 0 |
| ATOM | 1351 | C | ASP A 294 ASP A 294 | 246.772 -74.166 118.153 1.00 44.18 244.490 -76.064 114.323 1.00 42.63 | A | 0 |
| ATOM | 1352 | õ | ASP A 294 | 0.40 0.00 0.00 0.00 0.00 | A | C |
| MOTA | 1353 | N | TYR A 295 | 243.322 -76.434 114.275 1.00 40.46 245.168 -75.589 113.280 1.00 41.51 | A | 0 |
| ATOM | 1354 | CA | TYR A 295 | 244.534 -75.404 111.983 1.00 42.29 | A A | N C |
| ATOM | 1355 | CB | TYR A 295 | 245.046 -74.116 111.335 1.00 42.13 | A | C |
| ATOM | 1356 | CG | TYR A 295 | 245.120 -72.945 112.263 1.00 41.89 | A | c |
| ATOM | 1357 | CD1 | TYR A 295 | 246.211 -72.793 113.099 1.00 47.14 | A | Č |
| ATOM | 1358 | CE1 | TYR A 295 | 246.304 -71.731 113.973 1.00 47.33 | A | Ċ |
| MOTA | 1359 | | TYR A 295 | 244.117 -71.995 112.309 1.00 36.13 | A | С |
| MOTA | 1360 | | TYR A 295 | 244.212 -70.914 113.162 1.00 43.23 | A | С |
| MOTA | 1361 | CZ | TYR A 295 | 245.302 -70.785 113.996 1.00 47.19 | A | С |
| ATOM ATOM | 1362 1363 | OH C | TYR A 295 | 245.414 -69.690 114.838 1.00 57.32 | A | 0 |
| ATOM | 1364 | Ö | TYR A 295 TYR A 295 | 244.655 -76.563 110.985 1.00 41.49 244.224 -76.467 109.822 1.00 43.26 | A | C |
| ATOM | 1365 | N | LEU A 296 | | A | 0 |
| ATOM | 1366 | CA | LEU A 296 | 245.228 -77.668 111.448 1.00 39.99 245.411 -78.868 110.607 1.00 51.39 | A A | N |
| ATOM | 1367 | CB | LEU A 296 | 246.671 -79.611 111.016 1.00 53.81 | A | C C |
| MOTA | 1368 | CG | LEU A 296 | 248.033 -78.987 110.652 1.00 57.41 | Ā | c |
| ATOM | 1369 | | LEU A 296 | 249.165 -79.934 111.025 1.00 51.84 | A | c |
| ATOM | 1370 | CD2 | LEU A 296 | 248.040 -78.694 109.161 1.00 50.59 | A | Ċ |
| MOTA | 1371 | С | LEU A 296 | 244.205 -79.803 110.651 1.00 48.90 | A | С |
| ATOM | 1372 | 0 | LEU A 296 | 243.511 -79.890 111.645 1.00 60.00 | Α | 0 |
| ATOM | 1373 | N | PRO A 297 | 243.914 -80.480 109.550 1.00 49.64 | Α | N |
| ATOM | 1374 | CD | PRO A 297 | 244.428 -80.152 108.220 1.00 48.93 | A | С |
| ATOM ATOM | 1375 1376 | CA CB | PRO A 297 PRO A 297 | 242.782 -81.390 109.447 1.00 53.31 | A | С |
| ATOM | 1377 | CG | PRO A 297 | 242.450 -81.327 107.951 1.00 50.04 243.782 -81.194 107.367 1.00 48.93 | A | C |
| ATOM | 1378 | C | PRO A 297 | 0.40 4.00 0.00 0.00 | A | C |
| ATOM | 1379 | ŏ | PRO A 297 | 243.137 -82.762 109.966 1.00 57.23 244.303 -83.109 110.051 1.00 56.18 | A | C |
| ATOM | 1380 | N | PRO A 298 | 242.135 -83.562 110.334 1.00 59.72 | A A | O N |
| ATOM | 1381 | CD | PRO A 298 | 240.704 -83.237 110.308 1.00 64.33 | A | C |
| ATOM | 1382 | CA | PRO A 298 | 242.340 -84.917 110.853 1.00 62.61 | A | č |
| ATOM | 1383 | CB | PRO A 298 | 240.929 -85.463 110.920 1.00 65.22 | A | Č |
| ATOM | 1384 | CG | PRO A 298 | 240.143 -84.267 111.288 1.00 64.88 | A | Č |
| ATOM | 1385 | С | PRO A 298 | 243.245 -85.779 109.963 1.00 64.63 | A | Č |
| MOTA | 1386 | 0 | PRO A 298 | 244.184 -86.426 110.459 1.00 56.23 | A | 0 |
| ATOM | 1387 | N | GLU A 299 | 242.975 -85.781 108.656 1.00 60.03 | A | N |
| ATOM | 1388 | CA | GLU A 299 | 243.778 -86.574 107.711 1.00 58.56 | A | С |
| ATOM | 1389 | CB | GLU A 299 | 243.303 -86.339 106.265 1.00 57.01 | A | C |
| MOTA | 1390 | CG | GLU A 299 | 243.028 -84.864 105.914 1.00 52.94 | A | C |
| ATOM ATOM | 1391 1392 | CD OF1 | GLU A 299 | 241.596 -84.474 106.109 1.00 48.80 | A | C |
| 12 T OIA | 1326 | OFT | GLU A 299 | 241.003 -84.897 107.126 1.00 47.74 | A | 0 |
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| MOTA | 1463 | CD | GLU | A | 308 | 241.729 | -80.087 | 94.898 | 1.00 | 66.66 | P | C |
|--------------|------|--------|------|---|-----|---------|------------|---------|------|-------|------------|------|
| MOTA | 1464 | OE1 | GLU | A | 308 | 242.570 | | 94.305 | | 69.11 | P | |
| ATOM | 1465 | | ĠĿU | | | 240.722 | | 94.330 | | 69.49 | P | |
| MOTA | 1466 | С | GLU | | | 241.201 | | 99.802 | | 56.96 | P | |
| ATOM | 1467 | Ö | GLU | | | | -78.286 | | | 57.79 | P | |
| ATOM | 1468 | N | LYS | | | | -80.495 | | | 54.61 | A | |
| ATOM | 1469 | CA | LYS | | | | -80.332 | | | 54.70 | <i>P</i> | |
| MOTA | 1470 | CB | LYS | | | | -81.615 | | | 46.40 | P | |
| ATOM | 1471 | CG | LYS | | | | -81.859 | | | | | |
| | 1471 | | LYS | | | | -80.778 | | | 53.44 | P | |
| ATOM | | CD | | | | | | | | 58.61 | P | |
| ATOM | 1473 | CE | LYS | | | 235.600 | | 99.214 | | 60.43 | P | |
| ATOM | 1474 | NZ | LYS | | | | -80.026 | 99.209 | | 60.76 | P | |
| ATOM | 1475 | C | LYS | | | | -79.967 | | | 54.64 | P | |
| ATOM | 1476 | 0 | | | 309 | | -79.724 | | | 66.35 | P | |
| MOTA | 1477 | N | VAL | | | | -79.941 | | | 57.91 | . <i>P</i> | _ |
| MOTA | 1478 | CA | JAV | | | | -79.593 | | | 53.66 | P | |
| MOTA | 1479 | CB | VAL | | | | -79.974 | | | 52.18 | F | |
| ATOM | 1480 | | VAL | | | | -81.375 | | | 54.98 | | |
| MOTA | 1481 | CG2 | VAL | Α | 310 | 244.347 | -79.010 | 103.252 | 1.00 | 55.72 | F | |
| ATOM | 1482 | С | VAT | Α | 310 | | -78.091 | | 1.00 | 53.64 | F | A C |
| MOTA | 1483 | 0 | VAL | Α | 310 | | -77.638 | | 1.00 | 47.54 | P | . O |
| .ATOM | 1484 | N | ASP | Α | 311 | 242.008 | -77.332 | 103.168 | 1.00 | 50.01 | F | A N |
| MOTA | 1485 | CA | ASP | Α | 311 | 241.881 | -75.889 | 103.255 | 1.00 | 57.45 | I | A C |
| ATOM | 1486 | CB | ASP | А | 311 | 242.275 | -75.232 | 101.925 | 1.00 | 56.10 | P | . C |
| ATOM | 1487 | CG | ASP | Α | 311 | 243.756 | -75.367 | 101.624 | 1.00 | 55.84 | P | A C |
| MOTA | 1488 | OD1 | ASP | Α | 311 | 244.585 | -75.238 | 102.553 | 1.00 | 49.03 | P | A 0 |
| MOTA | 1489 | OD2 | ASP | Α | 311 | 244.085 | -75.597 | 100.453 | 1.00 | 54.46 | Į | A 0 |
| ATOM | 1490 | С | ASP | Α | 311 | 240.454 | -75.467 | 103.667 | 1.00 | 59.07 | F | A C |
| ATOM | 1491 | 0 | ASP | Α | 311 | 240.258 | -74.365 | 104.208 | 1.00 | 69.75 | I | . O |
| MOTA | 1492 | N | LEU | Α | 312 | 239.471 | -76.343 | 103.445 | 1.00 | 56.37 | Į | A N |
| ATOM | 1493 | CA | LEU | Α | 312 | 238.117 | -76.031 | 103.815 | 1.00 | 45.08 | Į | A C |
| MOTA | 1494 | СВ | LEU | Α | 312 | 237.135 | -76.975 | 103.126 | 1.00 | 46.93 | F | A C |
| ATOM | 1495 | ÇG | LEU | Α | 312 | 236.719 | -76.481 | 101.746 | 1.00 | 45.65 | F | 4 C |
| MOTA | 1496 | CD1 | LEU | Α | 312 | 236.262 | -77.698 | 100.966 | 1.00 | 57.08 | I | A C |
| ATOM | 1497 | CD2 | LEU | Α | 312 | 235.607 | -75.431 | 101.878 | | 42.14 | | A C |
| ATOM | 1498 | С | LEU | Α | 312 | | -76.204 | | | 42.72 | | A C |
| ATOM | 1499 | 0 | LEU | Α | 312 | 237.357 | -75.451 | 105.986 | | 41.50 | F | A 0 |
| MOTA | 1500 | N | TRP | Α | 313 | 238.778 | -77.211 | 105.814 | 1.00 | 35.13 | I | A N |
| ATOM | 1501 | CA | | | 313 | 238.818 | -77.454 | 107.257 | | 42.05 | F | A C |
| ATOM | 1502 | CB | | | 313 | | -78.718 | | | 37.59 | | A C |
| MOTA | 1503 | CG | TRP | Α | 313 | 239.903 | -78.960 | 108.973 | 1.00 | 37.21 | I | A C |
| MOTA | 1504 | CD2 | | | 313 | | -79.815 | | | 38.09 | | A C |
| ATOM | 1505 | CE2 | TRP | Α | 313 | | -79.742 | | 1.00 | 40.55 | | A C |
| MOTA | 1506 | CE3 | TRP | | | | -80.627 | | 1.00 | 42.38 | I | A C |
| MOTA | 1507 | CD1 | TRP | A | 313 | 240.895 | -78.418 | 109.716 | | 40.67 | F | A C |
| ATOM | 1508 | NE1 | TRP | Α | 313 | 240.843 | -78.885 | 111.022 | | 36.83 | 7 | |
| ATOM | 1509 | CZ2 | TRP | Α | 313 | 239.325 | -80.470 | 112.237 | 1.00 | 41.12 | P | C |
| ATOM | 1510 | | TRP | | | | -81.353 | | | 40.98 | | C |
| MOTA | 1511 | | TRP | | | | -81.265 | | | 42.79 | | C |
| ATOM | 1512 | С | | | 313 | 239.448 | -76.259 | 108.009 | | 45.03 | | A C |
| ATOM | 1513 | 0 | | | 313 | | -75.813 | | | 49.94 | F | |
| ATOM | 1514 | N | | | 314 | | -75.748 | | | 46.02 | | N |
| ATOM | 1515 | CA | | | 314 | | -74.624 | | | 41.93 | Ī | |
| ATOM | 1516 | CB | | | 314 | 242.523 | -74.354 | 107.341 | | 44.32 | F | |
| ATOM | 1517 | OG | | | 314 | | -75.505 | | | 38.93 | Ī | |
| MOTA | 1518 | C | | | 314 | | -73.392 | | | 39.99 | P | |
| ATOM | 1519 | ō | | | 314 | | -72.596 | | | 45.37 | Ī | |
| ATOM | 1520 | N | | | 315 | | -73.226 | | | 35.87 | P | |
| ATOM | 1521 | CA | | | 315 | | -72.091 | | | 35.10 | F | |
| MOTA | 1522 | CB | | | 315 | | -72.091 | | | 34.40 | P | |
| ATOM | 1523 | CG | | | 315 | | -70.872 | | | 41.64 | F | |
| ATOM | 1524 | | LEU | | | | -69.564 | | | 42.79 | P | |
| ATOM | 1525 | | LEU | | | | -71.022 | | | 40.03 | P | |
| ATOM | 1525 | CDZ | | | 315 | | -72.154 | | | 38.86 | P | |
| ATOM | 1527 | 0 | | | 315 | | -71.200 | | | 42.90 | P | |
| ATOM | 1528 | Ŋ | | | 316 | | -73.301 | | | 42.90 | P. | |
| | 1528 | CA | | | 316 | | -73.475 | | | 29.38 | P | |
| ATOM ATOM | 1529 | CA | | | 316 | | -73.475 | | | 38.31 | P. | |
| | 1530 | | | | 316 | | -72.317 | | | 44.99 | | |
| ATOM | 1531 | O N | | | | | -73.578 | | | 34.77 | P. P. | |
| ATOM | 1332 | 7.4 | A WT | Α | 317 | 230.233 | , 3. 3 , 6 | , | 1.00 | 34.// | P | , IA |

| ATOM | 1533 | CA | VAL | A | 317 | | 238.980 | -73.253 | 112.343 | 1.00 | 38.52 | A | С |
|--------------|--------------|-----------|-----|---|------------|---|---------|--------------------|---------|------|----------------|--------|--------|
| MOTA | 1534 | CB | VAL | | | | | -73.903 | | | 39.35 | A | С |
| ATOM | 1535 | | VAL | | | | | -73.322 | | | 39.07 | A | С |
| MOTA | 1536 | | VAL | | | | | -75.403 | | | 36.59 | A | C |
| ATOM | 1537 | С | VAL | | | | | -71.743 | | | 39.43 | A | Ç |
| ATOM ATOM | 1538 1539 | O N | | | 317 318 | | | -71.092 -71.195 | | | 39.97 | A. | N |
| MOTA | 1540 | CA | | | 318 | | | -69.769 | | | 35.94 35.49 | A A | C |
| MOTA | 1541 | CB | | | 318 | | | -69.443 | | | 34.72 | A | Č |
| ATOM | 1542 | CG | | | 318 | | | -68.678 | | | 35.85 | A | č |
| ATOM | 1543 | | LEU | | | | | -69.129 | | | 35.87 | A | Č |
| MOTA | 1544 | CD2 | LEU | Α | 318 | | 242.040 | ~68.906 | 108.254 | | 39.24 | A | С |
| MOTA | 1545 | С | | | 318 | | | -68.952 | | 1.00 | 41.79 | A | С |
| MOTA | 1546 | 0 | | | 318 | | | -67.943 | | | 36.26 | A | 0 |
| MOTA | 1547 | N | | | 319 | | | -69.398 | | | 35.62 | A | N |
| MOTA | 1548 | CA | | | 319 | | | -68.700 | | | 40.61 | A | C |
| ATOM ATOM | 1549 1550 | CB SG | | | 319 319 | | | -69.338 -68.489 | | | 35.35 | A A | c s |
| ATOM | 1551 | C | | | 319 | | | -68.734 | | | 25.40 35.51 | A A | C |
| ATOM | 1552 | ŏ | | | 319 | | | -67.810 | | | 40.27 | A | ő |
| ATOM | 1553 | N | | | 320 | | | -69.795 | | | 38.46 | A | N |
| ATOM | 1554 | CA | | | 320 | | 235.683 | -69.942 | 114.604 | | 39.25 | A | C |
| MOTA | 1555 | CB | TYR | Α | 320 | | 235.867 | -71.406 | 115.016 | 1.00 | 37.24 | A | С |
| ATOM | 1556 | CG | TYR | A | 320 | | | -71.683 | | 1.00 | 38.04 | A | С |
| MOTA | 1557 | | TYR | | | | | -71.333 | | | 34.91 | A | С |
| ATOM | 1558 | | TYR | | | | | -71.640 | | | 31.79 | A | С |
| MOTA | 1559 | | TYR | | | | | -72.331 -72.628 | | | 39.29 | A | C |
| ATOM ATOM | 1560 1561 | CEZ | TYR | | 320 | | | -72.289 | | | 35.49 41.97 | A. | C |
| ATOM | 1562 | OH | | | 320 | | | -72.575 | | | 35.00 | A A | o |
| ATOM | 1563 | C | | | 320 | | | -69.038 | | | 43.31 | A | č |
| MOTA | 1564 | 0 | | | 320 | | | -68.318 | | | 51.83 | A | ō |
| ATOM | 1565 | N | GLU | A | 321 | | 237.910 | -69.073 | 115.144 | 1.00 | 42.04 | A | N |
| MOTA | 1566 | CA | | | 321 | | | -68.249 | | | 43.24 | A | С |
| ATOM | 1567 | CB | | | 321 | | | -68.552 | | | 36.62 | A | С |
| ATOM | 1568 | CG | | | 321 | | | -67.733 | | | 43.20 | A | C |
| ATOM ATOM | 1569 1570 | CD OE1 | GLU | | 321 | | | -68.087 -69.101 | | | 47.61 49.19 | A | C |
| ATOM | 1571 | | GLU | | | | | -67.350 | | | 55.54 | A A | 0 |
| ATOM | 1572 | C | | | 321 | | | -66.763 | | | 42.47 | A | č |
| ATOM . | 1573 | 0 | GLU | Α | 321 | | 238.794 | -65.970 | 116.656 | | 48.77 | A | ō |
| MOTA | 1574 | N | | | 322 | | 238.073 | -66.377 | 114.539 | 1.00 | 40.79 | A | N |
| ATOM | 1575 | CA | | | 322 | | | -64.970 | | | 37.96 | A | С |
| ATOM | 1576 | CB | | | 322 | | | -64.737 | | | 37.47 | A | С |
| ATOM | 1577 1578 | CG CD1 | PHE | | 322 | | | -64.880 -64.729 | | | 39.59 | A | C |
| ATOM ATOM | 1579 | | PHE | | | | | -65.133 | | | 34.97 41.97 | A | C |
| ATOM | 1580 | | | | 322 | | | -64.830 | | | 36.15 | A A | C |
| MOTA | 1581 | | | | 322 | | | -65.232 | | | 35.10 | A | č |
| ATOM | 1582 | CZ | PHE | A | 322 | | | -65.081 | | | 38.47 | A | C |
| MOTA | 1583 | С | | | 322 | | 236.569 | -64.466 | 115.166 | | 40.06 | A | С |
| ATOM | 1584 | 0 | | | 322 | | | -63.305 | | | 37.07 | A | 0 |
| ATOM | 1585 | N | | | 323 | | | -65.356 | | | 34.80 | A | Ŋ |
| ATOM ATOM | 1586 1587 | CA CB | | | 323 323 | • | | -65.021 -65.873 | | | 30.32 | A | C |
| ATOM | 1588 | CG | | | 323 | | | -65.689 | | | 29.77 | A A | C |
| ATOM | 1589 | | | | 323 | | | -66.804 | | | 24.59 | A | c |
| ATOM | 1590 | | LEU | | | | | -64.288 | | | 30.36 | A | č |
| MOTA | 1591 | С | LEU | A | 323 | | 234.661 | -65.226 | 117.824 | | 40.81 | A | C |
| MOTA | 1592 | 0 | | | 323 | | | -64.495 | | | 36.74 | A | 0 |
| ATOM | 1593 | N | | | 324 | | | -66.247 | | | 38.37 | A | N |
| ATOM | 1594 | CA | | | 324 | | | -66.590 | | | 35.74 | A | C |
| MOTA MOTA | 1595 1596 | CB CG1 | LAV | | 324 | | | -68.102 -68.419 | | | 37.17 | A n | C |
| ATOM | 1597 | | VAL | | | | | -68.697 | | | 34.96 26.08 | A A | C |
| ATOM | 1598 | C | | | 324 | | | -66.012 | | | 35.95 | A | C |
| ATOM | 1599 | ō | | | 324 | | | -65.631 | | | 44.11 | A | ŏ |
| ATOM | 1600 | N | GLY | A | 325 | | | -65.929 | | | 41.01 | A | N |
| ATOM | 1601 | CA | GLY | | | | | -65.355 | | | 39.51 | A | С |
| MOTA | 1602 | С | GLY | A | 325 | | 240.283 | -66.402 | 119.960 | 1.00 | 44.55 | A | C |

| | | | | | | • | | |
|--------------|--------------|-----------|------------|---|------------|--|--------|--------|
| ATOM | 1603 | 0 | GLY | A | 325 | 241.414 -66.092 120.321 1.00 38.22 | A | 0 |
| ATOM | 1604 | | LYS | | | 239.929 -67.663 119.722 1.00 45.05 | A | N |
| ATOM | 1605 | | LYS | | | 240.881 -68.764 119.861 1.00 45.42 240.994 -69.180 121.325 1.00 52.62 | A A | C |
| ATOM ATOM | 1606 1607 | | LYS | | | 239.699 -69.600 121.927 1.00 55.78 | A | Ċ |
| ATOM | 1608 | | LYS | | | 239.856 -69.912 123.415 1.00 60.70 | A | С |
| ATOM | 1609 | | LYS | | | 238.486 -70.233 124.058 1.00 66.17 | A | C |
| MOTA | 1610 | NZ | LYS | | | 238.569 -70.651 125.479 1.00 62.77 | A | N |
| MOTA | 1611 | | LYS | | | 240.419 -69.937 119.005 1.00 46.11 239.259 -70.074 118.767 1.00 39.63 | A A | C |
| ATOM | 1612 1613 | O N | LYS PRO | | | 239.239 -70.074 118.767 1.00 39.63 | A | N |
| MOTA MOTA | 1614 | CD | PRO | | | 242.773 -70.850 118.901 1.00 43.78 | A | C |
| ATOM | 1615 | CA | PRO | | | 240.980 -71.968 117.726 1.00 41.74 | A | С |
| ATOM | 1616 | CB | PRO | | | 242.331 -72.631 117.446 1.00 38.86 | A | C |
| MOTA | 1617 | CG | PRO | | | 243.349 -71.561 117.738 1.00 42.00 | A A | C |
| MOTA | 1618 1619 | 0 | PRO PRO | | | 240.064 -72.895 118.474 1.00 40.42 240.166 -73.021 119.700 1.00 46.66 | A | 0 |
| ATOM ATOM | 1620 | N | | | 328 | 239.209 -73.624 117.743 1.00 40.91 | A | N |
| ATOM | 1621 | CD | | | 328 | 239.083 -73.540 116.278 1.00 35.93 | A | C |
| MOTA | 1622 | CA | PRO | A | 328 | 238.232 -74.572 118.297 1.00 43.34 | A | C |
| MOTA | 1623 | CB | | | 328 | 237.340 -74.900 117.106 1.00 40.94 | A | C |
| ATOM | 1624 | CG | | | 328 | 238.298 -74.799 115.948 1.00 38.83 238.785 -75.820 118.933 1.00 44.48 | A A | C C |
| MOTA | 1625 1626 | С О | | | 328 328 | 238.075 -76.507 119.657 1.00 56.46 | A | Ö |
| ATOM ATOM | 1627 | N | | | 329 | 240.053 -76.118 118.674 1.00 50.25 | A | N |
| ATOM | 1628 | CA | | | 329 | 240.691 -77.334 119.223 1.00 45.46 | A | C |
| MOTA | 1629 | CB | | | 329 | 241.119 -78.268 118.089 1.00 42.34 | A | C |
| ATOM | 1630 | CG | | | 329 | 240.026 -78.559 117.139 1.00 42.28 | A | C |
| ATOM | 1631 | | | | 329 | 238.895 -79.252 117.575 1.00 39.79 240.097 -78.138 115.808 1.00 39.80 | A A | C |
| MOTA MOTA | 1632 1633 | | PHE | | 329 329 | 237.824 -79.529 116.665 1.00 42.28 | A | č |
| ATOM | 1634 | | | | 329 | 239.034 -78.408 114.902 1.00 45.87 | A | С |
| ATOM | 1635 | CZ | | | 329 | 237.903 -79.106 115.332 1.00 40.12 | A | С |
| ATOM | 1636 | С | | | 329 | 241.904 -76.978 120.064 1.00 45.73 | A | C |
| MOTA | 1637 | 0 | | | 329 | 242.769 -77.808 120.277 1.00 40.30 241.958 -75.741 120.543 1.00 44.00 | A A | O N |
| ATOM ATOM | 1638 1639 | N CA | | | 330 330 | 243.070 -75.285 121.345 1.00 50.19 | A | C |
| MOTA | 1640 | CB | | | 330 | 242.855 -73.844 121.787 1.00 54.34 | A | č |
| ATOM | 1641 | CG | | | 330 | 244.140 -73.087 122.035 1.00 65.74 | A | С |
| ATOM | 1642 | CD | | | 330 | 243.932 -71.802 122.845 1.00 74.00 | A | C |
| ATOM | 1643 | | | | 330 | 244.822 -70.906 122.794 1.00 80.13 242.884 -71.701 123.543 1.00 77.27 | A A | 0 |
| ATOM ATOM | 1644 1645 | C C | | | 330 | 242.884 = 71.701 123.543 1.00 77.27 243.172 = 76.161 122.550 1.00 51.87 | A | c |
| ATOM | 1646 | Ö | | | 330 | 242.158 -76.668 123.029 1.00 54.61 | A | ō |
| ATOM | 1647 | N | | | 331 | 244.404 -76.359 123.020 1.00 56.85 | Α | N |
| MOTA | 1648 | CA | | | 331 | 244.680 -77.163 124.217 1.00 60.04 | A | C |
| MOTA | 1649 | CB | | | 331 | 244.791 -78.618 123.872 1.00 51.13 | A | C |
| MOTA | 1650 1651 | C O | | | 331 | 245.992 -76.676 124.795 1.00 60.84 246.630 -75.805 124.208 1.00 69.22 | A A | C |
| MOTA MOTA | 1652 | N | | | 332 | 246.378 -77.197 125.962 1.00 64.86 | A | N |
| ATOM | 1653 | CA | | | 332 | 247.637 -76.790 126.560 1.00 61.08 | A | C |
| ATOM | 1654 | CB | | | 332 | 247.514 -76.742 128.100 1.00 60.00 | A | C |
| MOTA | 1655 | CG | | | 332 | 246.822 -75.435 128.611 1.00 67.42 | A | C |
| ATOM | 1656 1657 | | | | 332 | 247.429 -74.359 128.654 1.00 68.56 245.547 -75.544 129.000 1.00 72.60 | A A | О И |
| ATOM ATOM | 1658 | C | | | 332 | 248.807 -77.666 126.080 1.00 60.05 | A | c |
| ATOM | 1659 | ō | | | 332 | 249.966 -77.257 126.234 1.00 65.40 | Α | Ó |
| ATOM | 1660 | N | THR | A | 333 | 248.512 -78.823 125.460 1.00 53.02 | A | N |
| MOTA | 1661 | CA | | | 333 | 249.562 -79.745 124.976 1.00 54.16 | A | C |
| MOTA | 1662 | CB | | | 333 | 249.652 -81.103 125.782 1.00 55.23 248.822 -82.111 125.160 1.00 53.00 | A A | C 0 |
| ATOM ATOM | 1663 1664 | | | | 333 | 249.296 -80.907 127.225 1.00 55.86 | A | C |
| ATOM | 1665 | C | | | 333 | 249.400 -80.153 123.497 1.00 59.22 | A | č |
| ATOM | 1666 | ŏ | | | 333 | 248.379 -79.845 122.897 1.00 59.44 | A | 0 |
| ATOM | 1667 | N | | | 334 | 250.358 -80.901 122.930 1.00 66.35 | A | N |
| ATOM | 1668 | CA | | | 334 | 250.331 -81.305 121.506 1.00 67.76 | A | C |
| ATOM | 1669 | CB | | | 334 | 251.770 -81.458 120.999 1.00 65.59 251.922 -82.193 119.636 1.00 60.98 | A A | C |
| ATOM ATOM | 1670 1671 | CG CD1 | | | 334 | 252.369 -81.519 118.539 1.00 58.37 | A | č |
| ATOM | 1672 | | | | 334 | 252.454 -82.152 117.323 1.00 57.12 | A | C |
| | | | | | | | | |

| ATOM | 1 673 | CD2 | TYR | A | 334 | 251.556 | -83.561 | 119.454 | 1.00 | 60.46 | | A | С |
|------|-------|-----|-----|---|-----|---------|---------|---------|------|-------|-----|----------|---|
| ATOM | 1674 | CE2 | TYR | Α | 334 | 251.612 | -84.203 | 118,235 | 1.00 | 54.51 | | A | С |
| ATOM | 1.675 | CZ | TYR | | | | -83.483 | | | 61.53 | | | c |
| | | OH | | | | | | | | | | A | |
| MOTA | 1676 | | TYR | | | | -84.054 | | | 64.63 | | A. | 0 |
| MOTA | 1677 | С | TYR | | | 249.706 | -82.673 | 121.408 | 1.00 | 72.76 | | A | С |
| ATOM | 1678 | 0 | TYR | Α | 334 | 249.561 | -83.257 | 120.347 | 1.00 | 80.80 | | A. | 0 |
| ATOM | 1679 | N | GLN | Α | 335 | 249,281 | -83.198 | 122.511 | | 75.82 | | A | N |
| MOTA | 1680 | CA | GLN | | | | -84.550 | | | 75.10 | | A | C |
| | | | | | | | | | | | | | |
| MOTA | 1681 | CB | GLN | | | | -85.260 | | | 74.39 | | A | С |
| ATOM | 1682 | CG | GLN | Ą | 335 | 251.326 | -84.889 | 123.021 | 1.00 | 71.11 | | A | C |
| ATOM | 1683 | CD | GLN | Α | 335 | 252.200 | -84.301 | 124.134 | 1.00 | 70.17 | | A | С |
| MOTA | 1684 | OE1 | GLN | Α | 335 | 253,434 | -84.204 | 123.959 | 1.00 | 71.56 | | A. | 0 |
| ATOM | 1685 | | GLN | | | | -83.897 | | | 67.14 | | | |
| | | | | | | | | | | | | A | И |
| ATOM | 1686 | С | | | 335 | | -84.426 | | | 72.12 | | A | С |
| MOTA | 1687 | 0 | GLN | A | 335 | 246.584 | -85.314 | 122.698 | 1.00 | 70.11 | | A. | 0 |
| MOTA | 1688 | N | GLU | Α | 336 | 247.129 | -83.272 | 123.527 | 1.00 | 67.17 | | A | N |
| ATOM | 1689 | CA | GLU | Α | 336 | 245.815 | -82.981 | 124,050 | 1,00 | 66.23 | | A | С |
| ATOM | 1690 | СВ | | | 336 | | -81.929 | | | 54.23 | | A | c |
| | | C | | | | | -82.389 | | | | | | |
| MOTA | 1691 | | | | 336 | | | | | 63.60 | | A | C |
| ATOM | 1692 | 0 | | | 336 | | -82.726 | | 1.00 | 68.92 | | A | 0 |
| MOTA | 1693 | N | THR | Α | 337 | 245.807 | -81.474 | 122.060 | 1.00 | 63.51 | | A | N |
| ATOM | 1694 | CA | THR | Α | 337 | 245.246 | -80.840 | 120.863 | 1.00 | 45.32 | | Α | С |
| MOTA | 1695 | CB | THR | Α | 337 | 246,221 | -79.805 | 120.292 | | 48.60 | | A | Ċ |
| ATOM | 1696 | | THR | | | | -78.730 | | | | | | |
| | | | | | | | | | | 44.49 | | A | 0 |
| MOTA | 1697 | | THR | | | | -79.262 | | 1.00 | 33.80 | | A | С |
| MOTA | 1698 | С | THR | Α | 337 | 245.031 | -81.916 | 119.825 | 1.00 | 55.74 | | A | С |
| MOTA | 1699 | 0 | THR | Α | 337 | 244.036 | -81.911 | 119.094 | 1.00 | 53.43 | | Α | 0 |
| ATOM | 1700 | N | TYR | Α | 338 | 245.979 | -82.848 | 119.758 | | 62.69 | | A | N |
| ATOM | 1701 | CA | | | 338 | | -83.948 | | | 62.09 | | A | c |
| | | CB | | | 338 | | | | | | | | |
| MOTA | 1702 | | | | | | -84.923 | | | 70.33 | | A | С |
| ATOM | 1703 | CG | | | 338 | 247.098 | -86.080 | 118.034 | 1.00 | 74.69 | | A | С |
| ATOM | 1704 | CD1 | TYR | Α | 338 | 248.041 | -86.116 | 117.016 | 1.00 | 72.79 | | A | С |
| ATOM | 1705 | CE1 | TYR | Α | 338 | 248.050 | -87.154 | 116.101 | 1.00 | 75.92 | | A | С |
| MOTA | 1706 | | TYR | | | | -87.121 | | | 70.94 | | Ą | č |
| ATOM | 1707 | | TYR | | | | -88.153 | | | | | | |
| | | | | | | | | | | 73.14 | | A | С |
| ATOM | 1708 | CZ | | | 338 | | -88.168 | | 1.00 | 73.24 | | A | С |
| ATOM | 1709 | ОН | TYR | Α | 338 | | -89.196 | | 1.00 | 74.46 | | A | 0 |
| ATOM | 1710 | С | TYR | Α | 338 | 244.586 | -84.698 | 118.971 | 1.00 | 62.03 | | A | С |
| ATOM | 1711 | 0 | TYR | A | 338 | | -85.017 | | | 52.46 | | A | Ō |
| ATOM | 1712 | N | | | 339 | | -84.991 | | | 58.53 | | A | N |
| | 1713 | | | | 339 | | -85.733 | | | | | | |
| MOTA | | CA | | | | | | | | 51.87 | | A | С |
| MOTA | 1714 | CB | | | 339 | | -86.042 | | 1.00 | 52.84 | | A | С |
| ATOM | 1715 | С | LYS | Α | 339 | 241.791 | -84.990 | 120.165 | 1.00 | 50.97 | , , | A | С |
| ATOM | 1716 | 0 | LYS | Α | 339 | 240.975 | -85.531 | 119.412 | 1.00 | 50.87 | | A | 0 |
| MOTA | 1717 | N | ARG | Α | 340 | 241.675 | -83.725 | 120.575 | | 44.05 | | A | N |
| ATOM | 1718 | CA | | | 340 | | -82.938 | | | 47.22 | | | |
| | | | | | | | | | | | | A. | C |
| ATOM | 1719 | CB | | | 340 | | -81.574 | | | 45.76 | | A. | С |
| ATOM | 1720 | CG | ARG | A | 340 | | -81.607 | | 1.00 | 52.85 | | A. | C |
| MOTA | 1721 | CD | ARG | Α | 340 | 240.241 | -80.202 | 122.999 | 1.00 | 59.79 | | A. | С |
| ATOM | 1722 | NE | ARG | A | 340 | 239.045 | -79.491 | 122.535 | 1.00 | 67.64 | | A | N |
| ATOM | 1723 | CZ | ARG | Α | 340 | | -78.186 | | | 65.86 | | A | C |
| ATOM | 1724 | | ARG | | | | -77.446 | | | 67.71 | | | |
| | 1725 | | | | | | | | | | | A. | N |
| ATOM | | | ARG | | | | -77.631 | | | 68.60 | | A. | N |
| ATOM | 1726 | С | | | 340 | | -82.765 | | 1.00 | 46.20 | | A. | С |
| ATOM | 1727 | 0 | ARG | A | 340 | 239.144 | -82.785 | 118.274 | 1.00 | 48.74 | | A | 0 |
| MOTA | 1728 | N | ILE | Α | 341 | 241.387 | -82.597 | 117.979 | | 47.52 | | A | N |
| ATOM | 1729 | CA | | | 341 | | -82.462 | | | 49.01 | | A | С |
| ATOM | 1730 | CB | | | 341 | | -82.067 | | | | | | |
| | | | | | | | | | | 48.35 | | A. | С |
| ATOM | 1731 | | ILE | | | | -82.130 | | | 34.18 | · · | A | С |
| MOTA | 1732 | CG1 | ILE | Α | 341 | 243.053 | -80.674 | 116.236 | 1.00 | 44.80 | | A | С |
| ATOM | 1733 | CD1 | ILE | Α | 341 | 244.317 | -80.259 | 115.592 | 1.00 | 47.34 | | A. | C |
| ATOM | 1734 | C | | | 341 | | -83.752 | | | 53.55 | | A | č |
| ATOM | 1735 | ŏ | | | 341 | | -83.734 | | | | | | |
| | | | | | | | | | | 44.79 | | A. | 0 |
| ATOM | 1736 | N | | | 342 | | -84.867 | | | 59.31 | | Ą | N |
| ATOM | 1737 | CA | SER | | | | -86.175 | | | 65.95 | 1 | Ą | C |
| ATOM | 1738 | CB | SER | A | 342 | | -87.227 | | 1.00 | 66.33 | | A. | С |
| MOTA | 1739 | OG | SER | Α | 342 | | -88.516 | | | 63.35 | | 4 | o |
| ATOM | 1740 | C | | | 342 | | -86.604 | | | 65.99 | | | |
| | | | | | | | | | | | | A | C |
| ATOM | 1741 | 0 | SER | | | | -87.327 | | | 61.18 | | 4 | 0 |
| ATOM | 1742 | N | ARG | A | 343 | 239.232 | -86.162 | 117.400 | 1.00 | 61.34 | ž | 4 | N |

| MOTA | 1743 | CA | ARG | Α | 343 | 237.910 | -86.478 | 117.932 | 1.00 | 59.46 | A | . C |
|------|--------------|-----|-----|---|-----|---------|--------------------|---------|------|-------|----------|-----|
| MOTA | 1744 | CB | ARG | Α | 343 | 237.888 | -86.410 | 119.456 | 1.00 | 58.77 | A | . С |
| MOTA | 1745 | CG | ARG | Α | 343 | 238.466 | -87.604 | 120.201 | 1.00 | 47.50 | A | . с |
| MOTA | 1746 | CD | ARG | A | 343 | 238.360 | -87.314 | 121.675 | 1.00 | 60.64 | A | C |
| ATOM | 1747 | NE | ARG | A | 343 | 238.972 | -88.327 | 122.530 | 1.00 | 66.55 | A | , N |
| ATOM | 1748 | CZ | ARG | Α | 343 | 238.930 | -88.278 | 123.865 | 1.00 | 74.36 | A | C |
| ATOM | 1749 | NH1 | ARG | Α | 343 | 238.309 | -87.268 | 124.510 | 1.00 | 73.84 | A | N |
| MOTA | 1750 | NH2 | ARG | A | 343 | 239.502 | -89.248 | 124.573 | 1.00 | 82.35 | A | . N |
| ATOM | 1751 | С | ARG | Α | 343 | | -85.448 | | 1.00 | 62.95 | P | . c |
| ATOM | 1752 | 0 | ARG | Α | 343 | 235.682 | -85.706 | 117.372 | | 61.25 | A | |
| ATOM | 1753 | N | VAL | Α | 344 | | -84.275 | | | 62.37 | A | |
| ATOM | 1754 | CA | VAL | Α | 344 | | -83.163 | | | 52.53 | Z. | |
| ATOM | 1755 | CB | | | 344 | | -83.614 | | | 46.83 | 7 | |
| ATOM | 1756 | | VAL | | | | -82.383 | | | 30.17 | A | |
| MOTA | 1757 | | VAL | | | | -84.445 | | | 41.05 | A | |
| ATOM | 1758 | С | | | 344 | | -82.735 | | | 56.35 | | |
| ATOM | 1759 | ō | | | 344 | | -82.790 | | | 58.20 | P | |
| ATOM | 1760 | N | | | 345 | | -82.345 | | | 52.70 | A | |
| MOTA | 1761 | CA | | | 345 | | -81.929 | | | 55.50 | A | |
| ATOM | 1762 | CB | | | 345 | | -82.610 | | | 59.39 | A | |
| ATOM | 1763 | CG | | | 345 | | -82.656 | | | 70.94 | P | |
| ATOM | 1764 | CD | | | 345 | | -83.623 | | | | | |
| MOTA | 1765 | | GLU | | | | | | | 80.37 | A | |
| | 1766 | | GLU | | | | -84.815 -83.190 | | | 83.68 | P | |
| ATOM | 1767 | | | | | | -80.414 | | | 84.85 | P | |
| ATOM | | C | | | 345 | | | · | | 55.94 | A | |
| ATOM | 1768 | 0 | | | 345 | | -79.866 | | | 52.34 | A | |
| ATOM | 1769 1770 | N | | | 346 | | -79.746 | | | 55.31 | A | |
| ATOM | | CA | | | 346 | | -78.298 | | | 58.97 | <i>P</i> | |
| ATOM | 1771 | CB | | | 346 | | -77.601 | | | 55.59 | A | |
| MOTA | 1772 | CG | | | 346 | | -77.671 | | | 51.30 | A | |
| ATOM | 1773 | | PHE | | | | -76.667 | | | 47.92 | A | |
| ATOM | 1774 | | PHE | | | | -78.734 | | | 51.74 | P | |
| ATOM | 1775 | | PHE | | | | -76.715 | | | 54.03 | A | |
| MOTA | 1776 | | PHE | | | | -78.810 | | | 54.32 | P | |
| ATOM | 1777 | CZ | | | 346 | | -77.803 | | | 51.48 | P | |
| ATOM | 1778 | С | | | 346 | | -77.832 | _ | | 60.04 | P | |
| ATOM | 1779 | 0 | | | 346 | | -78.494 | - | | 69.92 | P | |
| ATOM | 1780 | N | | | 347 | | -76.697 | | | 56.17 | A | |
| ATOM | 1781 | CA | | | 347 | | -76.158 | | | 54.44 | P | |
| ATOM | 1782 | CB | | | 347 | | -76.329 | | | 47.09 | A | |
| MOTA | 1783 | | THR | | | | -75.600 | | | 47.43 | A | |
| ATOM | 1784 | | THR | - | | | -77.783 | | | 48.24 | A | |
| ATOM | 1785 | C | | - | 347 | | -74.683 | | | 56.33 | A | |
| ATOM | 1786 | 0 | | | 347 | | -73.985 | | | 62.80 | A | - |
| MOTA | 1787 | N | | | 348 | | -74.235 | | | 63.69 | A | |
| ATOM | 1788 | CA | | _ | 348 | | -72.815 | | | 65.89 | A | _ |
| ATOM | 1789 | CB | | | 348 | | -72.558 | | | 57.72 | A | |
| ATOM | 1790 | CG | | | 348 | | -73.148 | | | 55.81 | A | |
| ATOM | 1791 | | PHE | | | | -74.364 | | | 51.99 | A | |
| ATOM | 1792 | | PHE | | | | -72.462 | | | 53.67 | P | |
| ATOM | 1793 | | PHE | | | | -74.857 | | | 46.52 | A | - |
| ATOM | 1794 | | PHE | | | | -72.966 | | | 50.86 | A | |
| ATOM | 1795 | CZ | | | 348 | | -74.166 | | | 51.38 | A | |
| ATOM | 1796 | C | | | 348 | | -72.048 | | | 65.81 | A | |
| ATOM | 1797 | 0 | | | 348 | | -72.532 | | | 73.51 | A | _ |
| MOTA | 1798 | N | | | 349 | | -70.898 | | | 59.06 | A | |
| ATOM | 1799 | CD | | | 349 | | -71.026 | | | 61.27 | A | |
| ATOM | 1800 | CA | | | 349 | | -69.933 | | | 56.66 | A | |
| MOTA | 1801 | CB | | | 349 | | -68.944 | | | 58.77 | A | |
| MOTA | 1802 | CG | | | 349 | | -69.875 | | | 55.14 | A | - |
| MOTA | 1803 | C | | | 349 | | -69.409 | | | 57.97 | A | |
| ATOM | 1804 | 0 | | | 349 | | -69.642 | | | 59.47 | A | . 0 |
| MOTA | 1805 | N | | | 350 | | -68.735 | | 1.00 | 59.19 | A | |
| MOTA | 1806 | CA | | | 350 | | -68.282 | | | 51.98 | A | |
| ATOM | 1807 | CB | | | 350 | | -67.819 | | 1.00 | 65.27 | A | C |
| ATOM | 1808 | CG | | | 350 | | -68.958 | | | 72.68 | A | C |
| MOTA | 1809 | | ASP | | | | -68.668 | | 1.00 | 77.91 | A | |
| MOTA | 1810 | OD2 | ASP | | | | -70.131 | | | 78.14 | A | |
| MOTA | 1811 | С | | | 350 | | -67.197 | | | 54.69 | A | С |
| ATOM | 1812 | 0 | ASP | A | 350 | 225.753 | -67.202 | 121.947 | 1.00 | 40.28 | A | 0 |
| | | | | | | | | | | | | |

| | | | | | | 51/75 | | |
|--------------|--------------|-----------|------------|----|------------|--|--------|--------|
| ATOM | 1813 | N | PHE | A | 351 | 227.786 -66.308 122.539 1.00 47.45 | A | N |
| MOTA | 1814 | CA | PHE | | | 227.682 -65.217 121.584 1.00 51.83 | A | C |
| MOTA | 1815 | CB | PHE | | | 228.693 -64.106 121.893 1.00 48.14 | A | C |
| MOTA MOTA | 1816 1817 | CG CD1 | PHE PHE | | | 230.108 -64.580 122.004 1.00 51.21 230.589 -65.111 123.207 1.00 49.73 | A A | C |
| ATOM | 1818 | | PHE | | | 230.979 -64.468 120.915 1.00 46.79 | A | Č |
| ATOM | 1819 | | PHE | | | 231.906 -65.506 123.312 1.00 48.51 | A | C |
| MOTA | 1820 | | PHE | A | 351 | 232.294 -64.864 121.026 1.00 47.18 | A | C |
| ATOM | 1821 | CZ | PHE | | | 232.758 -65.379 122.215 1.00 45.61 | A | C |
| ATOM | 1822 1823 | С 0 | PHE PHE | | | 227.797 -65.610 120.125 1.00 52.56 227.604 -64.771 119.250 1.00 57.29 | A A | C |
| MOTA MOTA | 1824 | N | VAL | | | 228.115 -66.874 119.863 1.00 54.95 | A | N |
| ATOM | 1825 | CA | VAL | | | 228.263 -67.341 118.495 1.00 48.00 | A | С |
| MOTA | 1826 | CB | VAL | | | 229.145 -68.621 118.432 1.00 43.19 | Α | С |
| ATOM | 1827 | | VAL | | | 229.300 -69.094 117.035 1.00 33.61 | A | C |
| ATOM ATOM | 1828 1829 | CG2 | VAL VAL | | | 230.509 -68.325 118.972 1.00 39.08 226.875 -67.603 117.916 1.00 48.25 | A A | C |
| ATOM | 1830 | 0 | VAL | | | 226.211 -68.567 118.255 1.00 51.46 | A | ō |
| ATOM | 1831 | N | THR | | | 226.446 -66.748 117.004 1.00 47.51 | A | N |
| MOTA | 1832 | CA | | | 353 | 225.122 -66.886 116.413 1.00 53.02 | A | C. |
| ATOM | 1833 | CB | | | 353 | 224.844 -65.817 115.383 1.00 47.94 225.671 -66.052 114.246 1.00 54.22 | A | 0 |
| MOTA MOTA | 1834 1835 | | THR THR | | | 225.671 -66.052 114.246 1.00 54.22 225.130 -64.437 115.950 1.00 47.89 | A A | c |
| ATOM | 1836 | C | | | 353 | 224.908 -68.227 115.753 1.00 52.60 | A | č |
| ATOM | 1837 | Ō | | | 353 | 225.851 -68.974 115.552 1.00 52.94 | A | 0 |
| ATOM | 1838 | N | | | 354 | 223.654 -68.513 115.404 1.00 55.25 | A | N |
| MOTA | 1839 | CA | | | 354 | 223.259 -69.786 114.819 1.00 56.40 221.736 -69.929 114.829 1.00 53.45 | A | C C |
| ATOM ATOM | 1840 1841 | CB C | | | 354 354 | 221.736 -69.929 114.829 1.00 53.45 223.762 -69.866 113.416 1.00 56.12 | A A | C |
| ATOM | 1842 | Ö | | | 354 | 224.078 -70.954 112.927 1.00 62.85 | A | ō |
| ATOM | 1843 | N | | | 355 | 223.831 -68.718 112.749 1.00 61.99 | A | N |
| ATOM | 1844 | CA | | | 355 | 224.317 -68.699 111.373 1.00 52.27 | A | C |
| ATOM | 1845 | C | | | 355 | 225.787 -69.093 111.250 1.00 52.90 | A | C |
| ATOM ATOM | 1846 1847 | N O | | | 355 356 | 226.166 -69.822 110.327 1.00 47.53 226.611 -68.602 112.182 1.00 47.86 | A A | N |
| ATOM | 1848 | CA | | | 356 | 228.022 -68.912 112.199 1.00 45.96 | A | c |
| ATOM | 1849 | CB | ALA | A | 356 | 228.721 -67.995 113.123 1.00 42.05 | A | С |
| MOTA | 1850 | C | | | 356 | 228.221 -70.359 112.627 1.00 47.72 | A | C |
| ATOM ATOM | 1851 1852 | O N | | | 356 357 | 229.011 -71.078 112.025 1.00 46.93 227.486 -70.784 113.651 1.00 49.03 | A A | O N |
| ATOM | 1853 | CA | | | 357 | 227.558 -72.153 114.146 1.00 56.76 | A | c |
| MOTA | 1854 | CB | ARG | Α | 357 | 226.549 -72.374 115.280 1.00 55.71 | A | С |
| ATOM | 1855 | CG | | | 357 | 226.876 -71.606 116.583 1.00 57.21 | A | С |
| ATOM | 1856 | CD | | | 357 | 226.018 -72.108 117.752 1.00 41.40 226.260 -71.310 118.928 1.00 43.14 | A | C |
| ATOM ATOM | 1857 1858 | NE CZ | ARG | | 357 357 | 226.260 -71.310 118.928 1.00 43.14 225.979 -71.698 120.148 1.00 39.58 | A A | N C |
| ATOM | 1859 | | ARG | | | 225.456 -72.893 120.340 1.00 42.66 | A | N |
| ATOM | 1860 | NH2 | ARG | | | 226.191 -70.869 121.163 1.00 51.41 | A | N |
| ATOM | 1861 | C | | | 357 | 227.299 -73.181 113.043 1.00 58.61 | A | C |
| ATOM ATOM | 1862 1863 | N O | | | 357 358 | 227.922 -74.260 112.996 1.00 62.70 226.383 -72.845 112.150 1.00 56.80 | A A | O N |
| ATOM | 1864 | CA | | | 358 | 226.053 -73.738 111.055 1.00 56.49 | A | Ç |
| ATOM | 1865 | CB | | | 358 | 224.792 -73.245 110.363 1.00 59.12 | A | C |
| ATOM | 1866 | CG | | | 358 | 224.380 -74.141 109.209 1.00 65.41 | A | С |
| ATOM | 1867 | | ASP | | | 224.036 -75.319 109.461 1.00 60.89 | A | 0 |
| MOTA | 1868 1869 | C CD2 | ASP | | 358 | 224.403 -73.669 108.049 1.00 68.71 227.178 -73.837 110.017 1.00 56.31 | A A | 0 |
| ATOM ATOM | 1870 | Ö | | | 358 | 227.523 -74.915 109.545 1.00 56.62 | A | Ö |
| ATOM | 1871 | N | | | 359 | 227.735 -72.694 109.640 1.00 57.58 | A | N |
| MOTA | 1872 | CA | | | 359 | 228.812 -72.663 108.658 1.00 55.45 | A | С |
| ATOM | 1873 | CB | | | 359 | 229.158 -71.227 108.302 1.00 53.49 | A | C |
| ATOM | 1874 1875 | CG CD1 | LEU | | 359 | 230.326 -71.029 107.344 1.00 49.10 230.077 -71.756 106.082 1.00 42.56 | A A | C |
| ATOM ATOM | 1876 | | LEU | | | 230.525 -69.538 107.083 1.00 51.15 | A | C |
| ATOM | 1877 | C | | | 359 | 230.048 -73.366 109.200 1.00 57.66 | A | Č |
| ATOM | 1878 | O | LEU | A | 359 | 230.680 -74.142 108.481 1.00 65.55 | A | 0 |
| MOTA | 1879 | N | | | 360 | 230.370 -73.121 110.470 1.00 49.19 | A | N |
| MOTA | 1880 | CA CB | | | 360 360 | 231.535 -73.740 111.089 1.00 43.07 231.819 -73.111 112.485 1.00 35.85 | A A | C |
| ATOM ATOM | 1881 1882 | | ILE | | | 232.892 -73.858 113.220 1.00 37.90 | Ā | C |
| -11 OI4 | 1002 | JU2 | ت ب ب | •• | | • | | _ |

| ATOM | 1883 | CG1 | ILE A | 360 | 232.254 - | -71.652 | 112.301 | 1.00 | 32.36 | Α | С |
|------|------|-----|-------|-----|-----------|---------|---------|------|-------|---|---|
| ATOM | 1884 | CD1 | ILE A | 360 | 232.250 - | -70-839 | 113.653 | 1.00 | 27.28 | A | С |
| ATOM | 1885 | C | ILE A | | 231.368 - | | | | 40.84 | A | č |
| | | | | | | | | | | | |
| MOTA | 1886 | 0 | ILE A | | 232.330 - | | | | 44.75 | A | 0 |
| ATOM | 1887 | N | SER A | | 230.158 - | - | | | 46.60 | Α | N |
| ATOM | 1888 | CA | SER A | 361 | 229.855 - | -77.089 | 111.780 | 1.00 | 52.65 | A | C |
| ATOM | 1889 | CB | SER A | 361 | 228.546 - | -77.265 | 112.526 | 1.00 | 49.78 | A | С |
| MOTA | 1890 | ŌG | SER A | 361 | 228.742 - | -77.062 | 113.925 | 1.00 | 60.97 | A | 0 |
| | | C | | | 229.827 - | | | | 53.49 | | Č |
| ATOM | 1891 | | SER A | | | | | | | A | |
| ATOM | 1892 | 0 | SER A | | 229.885 - | | | | 53.09 | A | 0 |
| MOTA | 1893 | N | ARG A | 362 | 229.799 - | -77.198 | 109.368 | 1.00 | 54.39 | A | N |
| MOTA | 1894 | CA | ARG A | 362 | 229.796 - | -77.841 | 108.066 | 1.00 | 52.12 | Α | С |
| ATOM | 1895 | CB | ARG A | 362 | 229.033 - | -76.978 | 107.065 | 1.00 | 59.93 | A | С |
| ATOM | 1896 | CG | ARG A | 362 | 227.535 - | | | | 61.75 | A | |
| | 1897 | CD | ARG A | | 226.887 - | | | | 69.51 | A | |
| MOTA | | | | | | | | | | | |
| ATOM | 1898 | NE | ARG A | | 225.432 - | | | | 76.19 | A | |
| ATOM | 1899 | CZ | ARG A | 362 | 224.625 - | -76.795 | 106.216 | 1.00 | 80.23 | A | С |
| ATOM | 1900 | NH1 | ARG A | 362 | 225.128 - | -77.919 | 105.716 | 1.00 | 81.25 | A | N |
| MOTA | 1901 | NH2 | ARG A | 362 | 223.313 - | -76.697 | 106.397 | 1.00 | 77.76 | А | N |
| ATOM | 1902 | С | ARG A | | 231.211 - | -78.066 | 107.537 | | 49.26 | А | |
| ATOM | 1903 | Ö | ARG A | | 231.460 - | | | | 49.03 | A | |
| | | | | | | | | | | | |
| ATOM | 1904 | N | LEU P | | 232.120 - | | | | 49.05 | A | |
| MOTA | 1905 | CA | LEU A | 363 | 233.493 - | -77.234 | 107.438 | 1.00 | 46.81 | A | С |
| ATOM | 1906 | CB | LEU P | 363 | 234.134 - | -75.850 | 107.508 | 1.00 | 42.60 | Α | С |
| ATOM | 1907 | CG | LEU A | 363 | 233.457 - | -74.729 | 106.714 | 1.00 | 44.53 | A | С |
| ATOM | 1908 | CD1 | LEU F | 363 | 234.050 - | -73.356 | 107.133 | | 43.18 | А | |
| ATOM | 1909 | | LEU P | | 233.602 | | | | 42.47 | A | |
| | | | | | | | | | | | |
| ATOM | 1910 | C | LEU F | | 234.270 - | | | | 49.03 | A | |
| ATOM | 1911 | 0 | LEU P | | 235.049 - | | | | 57.90 | А | 0 |
| MOTA | 1912 | N | LEU F | 364 | 234.062 - | -78.186 | 109.589 | 1.00 | 47.92 | A | N |
| ATOM | 1913 | CA | LEU A | 364 | 234.774 - | -79.071 | 110.488 | 1.00 | 49.66 | A | С |
| ATOM | 1914 | CB | LEU A | 364 | 234.792 - | -78.462 | 111.909 | 1.00 | 46.24 | A | С |
| ATOM | 1915 | CG | LEU F | | 235.511 - | | | | 47.59 | A | |
| | | | LEU F | | 235.230 | | | | | | |
| MOTA | 1916 | | | | | | | | 44.59 | A | |
| ATOM | 1917 | | LEU A | | 237.029 | | | | 45.40 | A | |
| ATOM | 1918 | С | LEU F | 364 | 234.233 - | -80.493 | 110.526 | 1.00 | 50.53 | A | C |
| ATOM | 1919 | 0 | LEU A | 364 | 233.804 - | -80.963 | 111.575 | 1.00 | 56.94 | А | 0 |
| ATOM | 1920 | N | LYS A | 365 | 234.267 | -81.178 | 109.385 | 1.00 | 61.00 | А | N |
| ATOM | 1921 | CA | LYS A | | 233.796 - | | | | 64.52 | A | |
| ATOM | 1922 | CB | | 365 | 233.059 | | | | 60.48 | A | |
| | | | LYS A | | | | | | | | |
| MOTA | 1923 | CG | | - | 231.753 | | | | 53.27 | A | |
| ATOM | 1924 | CD | LYS F | | 230.702 - | | | | 61.58 | A | |
| ATOM | 1925 | CE | LYS A | 365 | 229.295 · | | | 1.00 | 59.92 | A | C |
| ATOM | 1926 | NZ | LYS A | 365 | 228.297 - | -82.223 | 109.508 | 1.00 | 75.42 | A | N |
| MOTA | 1927 | С | LYS A | 365 | 235.026 - | -83.500 | 109.392 | 1.00 | 66.56 | А | С |
| ATOM | 1928 | 0 | LYS A | 365 | 236.146 · | | | | 71.71 | A | |
| ATOM | 1929 | N | HIS A | | 234.844 | | | | 68.20 | A | |
| | | | | | | | | | | | |
| ATOM | 1930 | CA | HIS A | | 236.011 | | | | 67.59 | A | |
| MOTA | 1931 | CB | HIS F | | 235.781 | | | | 66.12 | Α | |
| ATOM | 1932 | CG | HIS A | | 236.913 - | | | | 68.47 | Α | С |
| ATOM | 1933 | CD2 | HIS A | 366 | 237.810 - | -87.749 | 112.245 | 1.00 | 66.88 | Α | С |
| ATOM | 1934 | ND1 | HIS A | 366 | 237.332 - | -88.487 | 110.238 | 1.00 | 66.01 | A | N |
| ATOM | 1935 | CE1 | HIS A | 366 | 238.454 - | | | | 70.20 | A | C |
| ATOM | 1936 | | HIS A | | 238.761 - | | | | 64.97 | A | N |
| ATOM | 1937 | C | HIS A | | 236.184 | | | | 68.25 | | |
| | | | | | | | | | | A | C |
| MOTA | 1938 | 0 | HIS A | | 237.098 | | | | 74.87 | А | 0 |
| ATOM | 1939 | N | ASN A | | 235.262 - | | | | 65.45 | A | Ŋ |
| ATOM | 1940 | CA | ASN A | 367 | 235.379 · | -86.795 | 106.656 | 1.00 | 62.81 | Α | С |
| ATOM | 1941 | CB | ASN A | 367 | 234.189 - | -87.664 | 106.498 | 1.00 | 64.61 | A | С |
| MOTA | 1942 | CG | ASN A | 367 | 234.335 | -88.548 | 105.333 | 1.00 | 69.77 | Α | C |
| ATOM | 1943 | | ASN A | | 234.339 | | | | 65.35 | A | ő |
| | | | ASN A | | 234.518 - | | | | | | |
| ATOM | 1944 | | | | | | | | 69.27 | A | N |
| MOTA | 1945 | С | ASN A | | 235.504 - | | | | 60.17 | Α | С |
| MOTA | 1946 | 0 | ASN A | 367 | 234.685 - | | | | 67.65 | Α | 0 |
| ATOM | 1947 | N | PRO P | 368 | 236.650 - | -85.797 | 104.923 | 1.00 | 60.54 | Α | N |
| ATOM | 1948 | CD | PRO F | | 237.882 - | -86.364 | 105.504 | | 55.35 | A | C |
| ATOM | 1949 | CA | PRO F | | 236.981 - | | | | 55.82 | A | č |
| | | CB | PRO F | | 238.199 - | | | | 50.93 | A | c |
| ATOM | 1950 | | | | | | | | | | |
| ATOM | 1951 | CG | PRO F | | 238.938 - | | | | 54.85 | A | C |
| ATOM | 1952 | C | PRO P | 368 | 235.870 - | -84.741 | 102.783 | 1.00 | 59.90 | A | С |
| | | | | | | | | | | | |

| MOTA | 1953 | 0 | PRO | A | 368 | 235.706 -83.658 102.240 1.00 61.00 | A | 0 |
|--------------|--------------|----------|------------|---|----------------|--|--------|--------|
| MOTA | 1954 | N | SER | A | 369 | 235.093 -85.805 102.557 1.00 69.67 | A | N |
| ATOM | 1955 | CA | | | . 369 | 234.000 -85.800 101.588 1.00 72.88 | A | c |
| MOTA | 1956 | CB | | | 369 | 233.537 -87.237 101.347 1.00 75.22 | A | С |
| ATOM | 1957 | OG | | | . 369 | 234.654 -88.115 101.256 1.00 85.92 | A | 0 |
| ATOM | 1958 | C | | | 369 | 232.810 -84.951 102.046 1.00 71.84 | A | С |
| MOTA MOTA | 1959 1960 | O N | | | . 369 . 370 | 232.217 -84.231 101.229 1.00 75.53 | A | 0 |
| ATOM | 1961 | CA | | | 370 | 232.465 -85.039 103.333 | A | N |
| ATOM | 1962 | CB | | | 370 | | A | C |
| ATOM | 1963 | CG | | | 370 | 231.067 -84.743 105.296 1.00 64.15 230.629 -86.190 105.390 1.00 65.40 | A | C |
| MOTA | 1964 | CD | | | 370 | 230.923 -86.768 106.745 1.00 69.41 | A A | C |
| ATOM | 1965 | OE1 | GLN | A | 370 | 230.904 -86.051 107.752 1.00 75.34 | A | o |
| MOTA | 1966 | NE2 | GLN | A | 370 | 231.189 -88.073 106.792 1.00 63.71 | A | N |
| ATOM | 1967 | С | GLN | A | 370 | 231.551 -82.778 103.799 1.00 63.34 | A | c |
| ATOM | 1968 | 0 | | | 370 | 230.582 -82.028 103.608 1.00 65.90 | A | 0 |
| ATOM | 1969 | N | | | 371 | 232.802 -82.324 103.934 1.00 56.18 | A | N |
| ATOM | 1970 | CA | | | 371 | 233.085 -80.905 103.889 1.00 54.33 | Α | С |
| ATOM ATOM | 1971 | CB | | | 371 | 234.581 -80.691 103.961 1.00 48.64 | A | С |
| ATOM | 1972 1973 | CG CD | | | 371 | 235.109 -80.785 105.354 1.00 46.61 | A | C |
| ATOM | 1974 | NE | | | 371 | 236.618 -80.922 105.403 1.00 43.30 236.988 -81.971 106.350 1.00 42.51 | A | C |
| ATOM | 1975 | CZ | | | 371 | 000 000 00 100 100 | A | N |
| ATOM | 1976 | | ARG | | | 238.208 -82.476 106.436 1.00 42.45 239.165 -81.997 105.635 1.00 36.24 | A A | C |
| ATOM | 1977 | | ARG | | | 238.449 -83.494 107.266 1.00 33.74 | A | N N |
| ATOM | 1978 | С | ARG | A | 371 | 232.496 -80.275 102.651 1.00 56.25 | A | C |
| ATOM | 1979 | 0 | ARG | A | 371 | 232.578 -80.836 101.587 1.00 64.77 | A | Ö |
| ATOM | 1980 | N | PRO | A | 372 | 231.885 -79.089 102.783 1.00 60.04 | A | N |
| ATOM | 1981 | CD | | | 372 | 231.813 -78.305 104.029 1.00 57.31 | A | С |
| ATOM | 1982 | CA | | | 372 | 231.260 -78.365 101.659 1.00 57.19 | Α | С |
| ATOM | 1983 | CB | | | 372 | 230.522 -77.231 102.348 1.00 55.89 | A | С |
| ATOM ATOM | 1984 1985 | CG C | | | 372 372 | 231.448 -76.927 103.522 1.00 60.48 | A | С |
| ATOM | 1986 | 0 | | | 372 | 232.227 -77.848 100.593 1.00 59.74 233.424 -77.896 100.753 1.00 60.73 | A | C |
| ATOM | 1987 | N | | | 373 | 233.424 -77.896 100.753 | A. | 0 |
| ATOM | 1988 | CA | | | 373 | 232.482 -76.838 98.412 1.00 72.53 | A A | N C |
| ATOM | 1989 | CB | | | 373 | 231.763 -77.051 97.082 1.00 78.23 | A | C |
| ATOM | 1990 | CG | MET | A | 373 | 232.541 -77.969 96.165 1.00 91.60 | A | č |
| ATOM | 1991 | SD | | | 373 | 231.857 -78.033 94.463 1.00 92.28 | A. | s |
| ATOM | 1992 | CE | | | 373 | 230.337 -78.924 94.769 1.00 97.23 | A | С |
| ATOM ATOM | 1993 1994 | C | | | 373 | 232.631 -75.339 98.682 1.00 69.48 | A | С |
| ATOM | 1995 | O N | | | 373 374 | 231.861 -74.740 99.424 1.00 71.05 233.618 -74.722 98.060 1.00 66.97 | A | 0 |
| ATOM | 1996 | CA | | | 374 | | A | N |
| ATOM | 1997 | CB | | | 374 | 233.847 -73.303 98.261 1.00 65.90 235.155 -72.857 97.562 1.00 58.73 | A A | C |
| ATOM | 1998 | CG | | | 374 | 236.446 -73.311 98.258 1.00 51.64 | A | C |
| MOTA | 1999 | | LEU | | | 237.625 -73.104 97.321 1.00 47.33 | A | Č |
| ATOM | 2000 | | LEU | | | 236.629 -72.531 99.548 1.00 52.27 | A | Č |
| ATOM | 2001 | C | | | 374 | 232.660 -72.469 97.798 1.00 67.13 | A | С |
| MOTA | 2002 | 0 | | | 374 | 232.500 -71.320 98.219 1.00 75.20 | Α | 0 |
| ATOM ATOM | 2003 2004 | N CA | ARG | | 375 | 231.814 -73.025 96.939 1.00 67.09 | A | N |
| ATOM | 2005 | CB | | | 375 | 230.654 -72.254 96.482 1.00 63.14 230.122 -72.780 95.162 1.00 60.43 | A. | C |
| ATOM | 2006 | c | ARG | | | 230.122 -72.780 95.162 1.00 60.43 229.561 -72.275 97.541 1.00 63.36 | A | C |
| MOTA | 2007 | 0 | ARG | | | 228.882 -71.261 97.734 1.00 64.17 | A A | 0 |
| ATOM | 2008 | N | GLU | | | 229.413 -73.397 98.245 1.00 56.91 | A | И |
| MOTA | 2009 | CA | GLU | A | 376 | 228.404 -73.501 99.306 1.00 64.22 | A | Ċ |
| ATOM | 2010 | CB | GLU | | | 228.314 -74.947 99.815 1.00 67.11 | A | Ċ |
| ATOM | 2011 | CG | GLU | | | 227.797 -75.921 98.783 1.00 81.78 | A | С |
| ATOM | 2012 | CD | GLU | | | 228.016 -77.372 99.187 1.00 87.25 | A | С |
| ATOM ATOM | 2013 2014 | | GLU GLU | | | 229.137 -77.887 98.974 1.00 95.99 | A | 0 |
| ATOM | 2014 | C | GLU | | | 227.073 -78.001 99.732 1.00 98.67 | A | 0 |
| ATOM | 2015 | o | GLU | | | 228.791 -72.562 100.461 1.00 61.59 227.950 -72.145 101.275 1.00 63.73 | A. | C |
| ATOM | 2017 | N | VAL | | | 227.950 -72.145 101.275 1.00 63.73 230.078 -72.229 100.505 1.00 60.90 | A 2 | 0 |
| ATOM | 2018 | CA | VAL | | | 230.605 -71.361 101.539 1.00 60.11 | A A | С |
| ATOM | 2019 | CB | VAL | А | 377 | 232.149 -71.606 101.780 1.00 57.13 | A | C |
| MOTA | 2020 | | VAL | | | 232.701 -70.591 102.788 1.00 52.18 | A | c |
| MOTA | 2021 | | VAL | | | 232.364 -72.987 102.341 1.00 51.22 | A | č |
| MOTA | 2022 | С | VAL | A | 377 | 230.354 -69.928 101.140 1.00 59.92 | A | C |
| | | | | | | | | |

| MOTA | 2023 | 0 | VAL | A | 377 | 229.91 | .5 | -69.114 | 101.952 | 1.00 | 69.33 | | A | 0 |
|------|------|-------|----------------|----|-------|--------|-----|---------|---------|------|-------|---|----|---|
| ATOM | 2024 | N | LEU | | | | | -69.625 | 99.884 | _ | 54.97 | | A. | N |
| | | | | | | | | | | _ | | | | |
| ATOM | 2025 | CA. | LEU | | | | | -68.269 | 99.384 | | 57.61 | | Ą | C |
| MOTA | 2026 | CB | LEU | А | 378 | 231.17 | 8 | -68.090 | 98.026 | 1.00 | 55.37 | i | A. | С |
| ATOM | 2027 | CG | LEU | Α | 378 | 232.56 | 54 | -67.442 | 97.937 | 1.00 | 56.77 | | A | С |
| ATOM | 2028 | | LEU | | | | | -66.902 | 99.309 | | 59.47 | | Α. | Č |
| | | | | | | | | | | _ | | | | |
| ATOM | 2029 | CD2 | LEU | А | 378 | 233.51 | . 7 | -68.445 | 97.421 | 1.00 | 52.34 | | A. | C |
| MOTA | 2030 | С | LEU | Α | 378 | 228.99 | 95 | -67.925 | 99.248 | 1.00 | 53.77 | | A | С |
| MOTA | 2031 | 0 | LEU | Ζ. | 378 | 228 62 | 6 | -66.775 | 99.062 | 1.00 | 56.35 | | A | 0 |
| | | | | | | | | | | _ | | | | |
| ATOM | 2032 | N | GLU | | | | | -68.930 | 99.367 | | 58.84 | | A | N |
| MOTA | 2033 | CA. | ${f GLU}$ | A | 379 | 226.70 | 9 | -68.714 | 99.236 | 1.00 | 63.13 | | A | С |
| MOTA | 2034 | CB | GLU | Α | 379 | 226.10 | 1 | -69.720 | 98.274 | 1.00 | 65.30 | | Α | С |
| ATOM | 2035 | CG | GLU | Δ | 379 | 226.56 | 57 | -69.569 | 96.831 | 1.00 | 70.53 | | A | С |
| | | | | | | | | | | | | | | |
| MOTA | 2036 | CD | GLU | | | | | -70.533 | 95.895 | | 76.21 | | A | C |
| MOTA | 2037 | OE 1 | GLU | A, | 379 | 225.54 | 46 | -71.692 | 96.329 | 1.00 | 70.09 | | A | 0 |
| MOTA | 2038 | 0E 2 | GLU | Α | 379 | 225.5 | 47 | -70.124 | 94.737 | 1.00 | 76.09 | | A | 0 |
| ATOM | 2039 | С | GLU | Δ | 379 | 225.99 | 91 | -68.820 | 100.555 | 1.00 | 60.26 | | A | С |
| | | | GLU | | | | | -68.191 | | | 70.86 | | A | ō |
| MOTA | 2040 | 0 | | | | | | | | | | | | |
| MOTA | 2041 | N | \mathtt{HIS} | A | 380 | 226.5 | 35 | -69.606 | 101.468 | 1.00 | 54.34 | | A | N |
| ATOM | 2042 | CA. | HIS | Α | 380 | 225.93 | 21 | -69.775 | 102.771 | 1.00 | 54.61 | | A | С |
| MOTA | 2043 | СВ | HIS | А | 380 | 226.9 | 75 | -70.234 | 103.793 | 1.00 | 48.39 | | A | С |
| ATOM | | CG | | | 380 | | | -70.617 | | | 45.24 | | A | Č |
| | 2044 | | | | | | | | | | | | | |
| MOTA | 2045 | CD2 | HIS | A | 380 | | | ~71.793 | | 1.00 | 42.14 | | A | С |
| ATOM | 2046 | NDI | HIS | Α | 380 | 225.7 | 11 | -69.731 | 105.921 | 1.00 | 51.46 | | A | N |
| ATOM | 2047 | CE J. | HIS | А | 380 | 225.3 | 0.9 | -70.349 | 107.018 | 1.00 | 50.88 | | A | С |
| ATOM | 2048 | | HIS | | | | | -71.604 | | | 47.24 | | A | N |
| | | | | | | | | | - | - | | | | |
| MOTA | 2049 | С | | | 380 | | | -68.502 | | | 55.95 | | A | С |
| ATOM | 2050 | 0 | HIS | A | 380 | 225.8 | 07 | -67.409 | 103.206 | 1.00 | 60.83 | | A | 0 |
| ATOM | 2051 | N | PRO | Α | 381 | 223.9 | 70 | -68.630 | 103.727 | 1.00 | 55.60 | | A | N |
| ATOM | 2052 | CD | | | 381 | | | -69.910 | | | 51.69 | | A | С |
| | | | | | | | | | | | | | | |
| atom | 2053 | CA | | | 381 | | | -67.522 | | | 53.48 | | A | C |
| ATOM | 2054 | CB | | | 381 | 221.9 | 97 | -68.257 | 104.936 | 1.00 | 49.53 | | A | С |
| ATOM | 2055 | CG | PRO | Α | 381 . | 221.8 | 20 | -69.442 | 104.035 | 1.00 | 49.24 | | A | С |
| MOTA | 2056 | C | | | 381 | | | -66.545 | | | 56.98 | | A | С |
| | | | | | | | | | | | | | | |
| ATOM | 2057 | 0 | | | 381 | | | -65.320 | | | 59.03 | | A | 0 |
| ATOM | 2058 | N | TRP | Α | 382 | 224.6 | 35 | -67.091 | 106.164 | 1.00 | 54.77 | | A | N |
| ATOM | 2059 | CA | TRP | Α | 382 | 225.3 | 40 | -66.282 | 107.146 | 1.00 | 55.06 | | A | С |
| MOTA | 2060 | CB | TRP | A | 382 | 225.9 | 71 | -67.165 | 108,240 | 1.00 | 54.64 | | A | C |
| ATOM | 2061 | CG | | | 382 | | | -66.368 | | | 55.47 | | A | c |
| | | | | | | | | | | | | | | |
| ATOM | 2062 | CD2 | | | 382 | | | -66.195 | | | 58.05 | | A | С |
| ATOM | 2063 | CE2 | TRP | Α | 382 | 228.3 | 44 | -65.342 | 110.476 | 1.00 | 60.80 | | A | C |
| ATOM | 2064 | CE3 | TRP | Α | 382 | 229.2 | 10 | -66.680 | 108.649 | 1.00 | 60.95 | | A | С |
| ATOM | 2065 | CD1 | | | 382 | | | -65.634 | | | 58.89 | | A | С |
| | | | | | | | | -65.011 | | | | | | |
| ATOM | 2066 | NE1 | | | 382 | | - | | | | 59.37 | | A | N |
| MOTA | 2067 | cz2 | TRP | Α | 382 | 229.6 | 32 | -64.965 | 110.871 | 1.00 | 64.01 | | A | С |
| ATOM | 2068 | CZ3 | TRP | Α | 382 | 230.4 | 91 | -66.302 | 109.042 | 1.00 | 60.80 | | A | С |
| ATOM | 2069 | CH2 | TRP | А | 382 | 230.6 | 88 | -65.458 | 110.140 | 1.00 | 65.05 | | Α | С |
| ATOM | 2070 | C | | | 382 | | | -65.476 | | | 50.36 | | A | c |
| | | | | | | | - | | | | | | | |
| MOTA | 2071 | 0 | | | 382 | | | -64.300 | | | 56.46 | | A | 0 |
| ATOM | 2072 | N | ILE | A | 383 | 227.0 | 94 | -66.115 | 105.527 | 1.00 | 50.17 | | A | N |
| ATOM | 2073 | CA | ILE | Α | 383 | 228.1 | 63 | -65.454 | 104.757 | 1.00 | 51.21 | | A | С |
| MOTA | 2074 | CB | TLE | А | 383 | 228.9 | 14 | -66.460 | 103.856 | 1.00 | 42.86 | | A | С |
| | | CG2 | | | 383 | | | -65.709 | | | | | A | |
| ATOM | 2075 | | | | | | | | | _ | 42.15 | | | C |
| ATOM | 2076 | CG1 | | | 383 | | | -67.329 | | | 40.04 | | A | С |
| ATOM | 2077 | CD1 | ILE | Α | 383 | 230.9 | 43 | -66.520 | 105.429 | 1.00 | 40.46 | | A | С |
| MOTA | 2078 | С | ILE | Α | 383 | 227.6 | 59 | -64.305 | 103.873 | 1.00 | 52.36 | | A | С |
| ATOM | 2079 | 0 | | | 383 | | | -63.229 | | | 51.23 | | A | 0 |
| | | | | | | | | -64.533 | | | | | | |
| ATOM | 2080 | N | | | 384 | | | | | | 54.23 | | A | N |
| ATOM | 2081 | CA | THR | Α | 384 | | | -63.535 | | | 58.09 | | A | С |
| MOTA | 2082 | CB | THR | Α | 384 | 225.0 | 46 | -64.197 | 101.265 | 1.00 | 57.25 | | A | C |
| ATOM | 2083 | OG1 | | | 384 | 224.3 | 20 | -65.235 | 101.920 | 1.00 | 65.44 | | A | 0 |
| | 2084 | CG2 | | | 384 | | | -64.804 | | | 59.94 | | A | č |
| ATOM | | | | | | | | | | | | | | |
| ATOM | 2085 | С | | | 384 | | | -62.436 | | | 57.62 | | A | С |
| MOTA | 2086 | 0 | THR | Α | 384 | 224.9 | 29 | -61.395 | 102.420 | 1.00 | 61.64 | | Α | 0 |
| ATOM | 2087 | N | ALA | Α | 385 | 224.9 | 11 | -62.655 | 104.249 | 1.00 | 60.34 | | A | N |
| ATOM | 2088 | CA | | | 385 | | | -61.658 | | | 57.14 | | A | C |
| | | | | | | | | | | | | | | |
| ATOM | 2089 | CB | | | 385 | | | -62.376 | | | 61.04 | | Α. | C |
| ATOM | 2090 | С | | | 385 | | | -60.735 | | | 57.68 | | A. | С |
| ATOM | 2091 | 0 | ALA | Α | 385 | 224.6 | 44 | -59.765 | 106.467 | 1.00 | 56.76 | | A | 0 |
| ATOM | 2092 | N | | | 386 | 226.4 | 05 | -61.038 | 105.919 | | 57.22 | | A | N |
| | _002 | | | | | | _ | • | | | | | - | |

| ATOM | 2093 | CA | ASN | A | 386 | 227.312 -60.217 106.705 1.00 59.50 | A | C |
|--------------|--------------|----------|------------|---|------------|--|--------|---------|
| ATOM | 2094 | CB | ASN | A | 386 | 227.751 -60.993 107.939 1.00 58.18 | A | C |
| ATOM | 2095 | CG | ASN | Α | 386 | 226.583 -61.313 108.874 1.00 60.78 | A | C |
| MOTA | 2096 | | ASN | | | 226.026 -60.419 109.536 1.00 55.54 | A | 0 |
| MOTA | 2097 | ND2 | | | | 226.201 -62.591 108.923 1.00 55.70 | A | N |
| ATOM | 2098 | С | ASN | | | 228.540 -59.733 105.965 1.00 55.04 | A | C |
| MOTA | 2099 | 0 | ASN | | | 229.128 -58.723 106.336 1.00 58.67 | A. | 0 |
| MOTA | 2100 | N | | | 387 | 228.903 -60.444 104.906 1.00 58.95 | A | N |
| MOTA | 2101 | CA | | | 387 | 230.095 -60.110 104.132 1.00 63.83 | A | C |
| ATOM | 2102 | CB | | | 387 | 230.472 -61.278 103.220 1.00 55.03 | A | C |
| ATOM | 2103 | OG | | | 387 | 231.719 -61.061 102.599 1.00 57.80 | A | 0 |
| MOTA | 2104 | C | | | 387 | 229.865 -58.867 103.278 1.00 64.86 | A | С 0 |
| ATOM | 2105 | 0 | | | 387 388 | 228.745 -58.607 102.826 1.00 68.20 230.916 -58.091 103.063 1.00 67.77 | A A | Ŋ |
| ATOM | 2106 | N C7 | | | 388 | 230.786 -56.912 102.251 1.00 71.39 | A | C |
| MOTA | 2107 2108 | CA CB | | | 388 | 231.430 -55.722 102.969 1.00 71.24 | A | Ċ |
| ATOM ATOM | 2109 | OG | | | 388 | 232.815 -55.916 103.141 1.00 79.50 | A | ŏ |
| ATOM | 2110 | C | | | 388 | 231.403 -57.150 100.872 1.00 71.24 | A | č |
| MOTA | 2111 | Ö | | | 388 | 231.024 -56.501 99.909 1.00 76.22 | A | ŏ |
| ATOM | 2112 | N | | | 389 | 232.336 -58.091 100.767 1.00 70.18 | A | N |
| MOTA | 2113 | CA | | | 389 | 232.951 -58.347 99.475 1.00 67.46 | A | C |
| MOTA | 2114 | CB | LYS | | | 234.459 -58.686 99.667 1.00 49.89 | A | C |
| MOTA | 2115 | C | | | 389 | 232.216 -59.459 98.688 1.00 68.81 | A | C |
| ATOM | 2116 | 0 | LYS | A | 389 | 231.441 -60.236 99.337 1.00 76.61 | Α | 0 |
| ATOM | 2117 | OXT | LYS | A | 389 | 232.453 -59.564 97.435 1.00 76.72 | Α | 0 |
| MOTA | 2118 | PB | ADP | s | 531 | 257.416 -68.553 107.649 1.00 34.84 | s | P |
| MOTA | 2119 | 01B | ADP | S | 531 | 258.545 -67.776 107.191 1.00 50.81 | S | 0 |
| MOTA | 2120 | 02B | ADP | S | 531 | 257.209 -69.880 106.879 1.00 48.35 | s | 0 |
| MOTA | 2121 | O3B | ADP | S | 531 | 257.422 -68.756 109.226 1.00 53.79 | s | 0 |
| MOTA | 2122 | PA | ADP | | | 256.077 -66.204 106.616 1.00 35.25 | S | P |
| MOTA | 2123 | | ADP | | | 256.842 -66.123 105.373 1.00 33.66 | S | 0 |
| MOTA | 2124 | | | | 531 | 254.551 -65.860 106.461 1.00 54.13 | S | 0 |
| ATOM | 2125 | | | | 531 | 256.162 -67.643 107.261 1.00 62.78 | S | 0 |
| MOTA | 2126 | | | | 531 | 256.892 -65.243 107.657 1.00 48.32 | S | 0 |
| ATOM | 2127 | | ADP | | | 256.442 -65.218 109.085 1.00 61.70 255.856 -63.898 109.556 1.00 46.54 | s s | C |
| MOTA MOTA | 2128 2129 | 04* | ADP ADP | | | 255.856 -63.898 109.556 1.00 46.54 256.542 -62.868 108.818 1.00 44.98 | S | o |
| MOTA | 2130 | | | | 531 | 254.372 -63.620 109.292 1.00 37.55 | s | Č |
| ATOM | 2131 | | | | 531 | 253.658 -64.161 110.347 1.00 46.23 | s | ō |
| ATOM | 2132 | | | | 531 | 254.337 -62.080 109.181 1.00 46.36 | s | Ċ |
| ATOM | 2133 | | ADP | | | 254.148 -61.399 110.423 1.00 42.59 | S | Ó |
| ATOM | 2134 | C1* | ADP | S | 531 | 255.710 -61.716 108.597 1.00 43.16 | s | С |
| ATOM | 2135 | N9 | ADP | S | 531 | 255.666 -61.436 107.162 1.00 48.23 | S | N |
| ATOM | 2136 | C8 | ADP | S | 531 | 255.946 -62.302 106.136 1.00 47.43 | S | С |
| MOTA | 2137 | N7 | ADP | S | 531 | 255.811 -61.734 104.897 1.00 42.83 | S | N |
| ATOM | 2138 | C5 | | | 531 | 255.418 -60.464 105.177 1.00 40.36 | s | С |
| ATOM | 2139 | C6 | | | 531 | 255.122 -59.337 104.279 1.00 44.75 | S | С |
| ATOM | 2140 | И6 | | | 531 | 255.151 -59.400 102.949 1.00 22.67 | s | N |
| MOTA | 2141 | N1 | | | 531 | 254.762 -58.153 104.964 1.00 40.38 | s | N |
| ATOM | 2142 | C2 | | | 531 | 254.725 -58.057 106.364 1.00 50.55 | S | C |
| ATOM | 2143 | N3 | | | 531 | 254.992 -59.070 107.188 1.00 51.07 | S | И |
| MOTA | 2144 | C4 MG | MG2 | | 531 1 | 255.351 -60.245 106.574 1.00 46.49 254.502 -68.175 108.413 1.00 47.20 | s X | C MG |
| ATOM | 2145 2146 | MG | MG2 | | | 255.864 -71.389 106.282 1.00 52.14 | X | MG |
| ATOM ATOM | 2140 | | WAT | | | 264.531 -71.881 94.078 1.00 38.88 | W | 0 |
| MOTA | 2148 | | WAT | | | 242.403 -78.272 113.237 1.00 54.89 | W | ő |
| ATOM | 2149 | | WAT | | | 232.705 -62.634 117.460 1.00 37.08 | W | Ö |
| ATOM | 2150 | | WAT | | | 251.977 -73.020 102.685 1.00 62.00 | W | ő |
| ATOM | 2151 | | WAT | | | 275.163 -72.604 97.774 1.00 53.95 | W | ŏ |
| MOTA | 2152 | | TAW | | | 232.526 -85.909 111.573 1.00 35.05 | W | ō |
| MOTA | 2153 | | WAT | | | 259.170 -71.102 103.608 1.00 40.42 | W | 0 |
| MOTA | 2154 | | WAT | | | 249.904 -55.205 99.315 1.00 26.87 | W | 0 |
| ATOM | 2155 | OH2 | WAT | W | 9 | 229.701 -63.236 117.265 1.00 25.50 | W | 0 |
| | | | | | | | | |

Fig. 6

| Table B | | | | | | | | | | | |
|--------------|----------|----------|------------|---|------------|---------|--------------------|------------------|--------------------------|--------|--------|
| ATOM | 1 | СВ | SER | Α | 123 | 174.078 | 193.853 | 20.627 | 1.00 33.78 | А | С |
| ATOM | 2 | OG | | | 123 | | 193.080 | 21.584 | 1.00 34.86 | A | ō |
| ATOM | 3 | С | SER | A | 123 | | 195.751 | 21.954 | 1.00 32.28 | A | C |
| ATOM | 4 | 0 | SER | A | 123 | | 196.187 | 22.580 | 1.00 32.38 | A | 0 |
| ATOM | 5 | N | SER | A | 123 | 174.192 | 196.109 | 19.556 | 1.00 32.09 | A | N |
| MOTA | 6 | CA | SER | A | 123 | | 195.246 | 20.532 | 1.00 33.80 | A | С |
| MOTA | 7 | N | | | 124 | | 195.682 | 22.463 | 1.00 30.56 | A | N |
| ATOM | 8 | CA | | | 124 | | 196.059 | 23.849 | 1.00 31.07 | A | С |
| ATOM | 9 | CB | | | 124 | | 196.727 | 24.005 | 1.00 31.64 | A | С |
| ATOM | 10 | CG | | | 124 | | 197.847 | 23.021 | 1.00 33.77 | A | C |
| ATOM | 11 12 | CD | | | 124 | | 198.157 | 22.847 | 1.00 35.14 | A | C |
| MOTA MOTA | 13 | CE NZ | | | 124 124 | | 198.989 | 21.582 21.123 | 1.00 38.52 1.00 40.74 | A | С N |
| ATOM | 14 | C | | | 124 | | 194.785 | 24.714 | 1.00 40.74 | A A | C |
| ATOM | 15 | Ö | | | 124 | | 194.845 | 25.913 | 1.00 30.29 | A | Ö |
| MOTA | 16 | N | | | 125 | | 193.646 | 24.102 | 1.00 30.71 | A | N |
| MOTA | 17 | CA | | | 125 | | 192.375 | 24.835 | 1.00 29.50 | A | C |
| ATOM | 18 | СВ | LYS | Α | 125 | 171.942 | 191.210 | 23.951 | 1.00 32.42 | A | С |
| ATOM | 19 | CG | LYS | Α | 125 | 170.496 | 191.147 | 23.609 | 1.00 35.74 | A | С |
| ATOM | 20 | CD | LYS | Α | 125 | 170.221 | 189.915 | 22.777 | 1.00 38.96 | A | С |
| MOTA | 21 | CE | | | 125 | | 189.905 | 22.351 | 1.00 44.54 | Α | С |
| ATOM | 22 | NZ | | | 125 | | 188.576 | 21.807 | 1.00 44.21 | A | N |
| ATOM | 23 | C | | | 125 | | 192.027 | 25.381 | 1.00 26.48 | A | C |
| ATOM ATOM | 24 25 | о И | | | 125 126 | | 192.438 | 24.859 | 1.00 24.13 | A | 0 |
| ATOM | 26 | CA | | | 126 | | 190.756 | 26.421 27.020 | 1.00 24.15 1.00 22.33 | A A | N C |
| ATOM | 27 | CB | | | 126 | | 189.835 | 28.191 | 1.00 22.33 | A | c |
| MOTA | 28 | CG | | | 126 | | 189.331 | 28.897 | 1.00 18.73 | A | c |
| ATOM | 29 | CD | | | 126 | | 188.263 | 29.847 | 1.00 19.74 | A | č |
| ATOM | 30 | NE | ARG | Α | 126 | 176.552 | 187.628 | 30.420 | 1.00 16.73 | A | N |
| ATOM | 31 | CZ | ARG | A | 126 | 176.503 | 186.741 | 31.394 | 1.00 17.59 | A | С |
| MOTA | 32 | | ARG | | | | 186.391 | 31.902 | 1.00 16.71 | A | N |
| ATOM | 33 | | ARG | | | | 186.214 | 31.854 | 1.00 18.45 | A | N |
| ATOM | 34 | C | | | 126 | | 189.995 | 25.943 | 1.00 22.44 | A | C |
| ATOM ATOM | 35 36 | И | | | 126 127 | | 189.077 | 25.296 25.763 | 1.00 20.29 | A | 0 |
| ATOM | 37 | CA | | | 127 | | 189.815 | 24.787 | 1.00 21.10 1.00 19.12 | A A | N C |
| ATOM | 38 | СВ | | | 127 | | 190.934 | 24.102 | 1.00 18.99 | A | c |
| ATOM | 39 | CG | | | 127 | | 191.925 | 23.355 | 1.00 15.64 | A | Č |
| ATOM | 40 | CD | GLN | A | 127 | | 191.297 | 22.162 | 1.00 17.04 | A | č |
| ATOM | 41 | OE1 | GLN | A | 127 | 177.748 | 191.151 | 21.093 | 1.00 21.45 | A | 0 |
| ATOM | 42 | | GLN | | | | 190.912 | 22.339 | 1.00 20.66 | A | N |
| MOTA | 43 | C | | | 127 | | 188.861 | 25.496 | 1.00 17.70 | A | С |
| ATOM ATOM | 44 | 0 | | | 127 | | 188.941 | 26.715 | 1.00 13.46 | A | 0 |
| ATOM | 45 46 | N CA | | | 128 128 | | 187.956 187.014 | 24.735 25.303 | 1.00 16.62 1.00 14.25 | A | N |
| ATOM | 47 | CB | | | 128 | | 186.029 | 24.237 | 1.00 14.23 | A A | C |
| ATOM | 48 | CG | | | 128 | | 185.060 | 23.779 | 1.00 9.34 | Ā | C |
| ATOM | 49 | | TRP | | | | 184.022 | 24.557 | 1.00 13.44 | A | č |
| ATOM | 50 | CE2 | TRP | Α | 128 | 178.396 | 183.304 | 23.704 | 1.00 11.84 | A | č |
| ATOM | 51 | | TRP | | | 179.389 | 183.618 | 25.899 | 1.00 15.05 | A | C |
| ATOM | 52 | CD1 | TRP | A | 128 | | 184.945 | 22.529 | 1.00 11.79 | A | С |
| ATOM | 53 | | TRP | | | | 183.893 | 22.469 | 1.00 12.24 | A | N |
| ATOM | 54 | | TRP | | | | 182.204 | 24.146 | 1.00 10.99 | A | C |
| ATOM | 55 56 | | TRP TRP | | | | 182.523 181.828 | 26.336 | 1.00 15.81 | A | C |
| ATOM ATOM | 57 | Cnz | | | 128 | | 187.777 | 25.457 25.855 | 1.00 13.35 1.00 16.17 | A | C |
| ATOM | 58 | o | | | 128 | | 188.903 | 25.457 | 1.00 16.17 | A A | C |
| ATOM | 59 | N | ALA | | | | 187.146 | 26.790 | 1.00 17.40 | A | N |
| ATOM | 60 | CA | ALA | | | | 187.695 | 27.415 | 1.00 17.26 | A | Ċ |
| ATOM | 61 | СВ | | | 129 | | 188.595 | 28.576 | 1.00 8.15 | A | Ċ |
| ATOM | 62 | С | ALA | | | | 186.478 | 27.906 | 1.00 17.06 | A | С |
| ATOM | 63 | 0 | ALA | Α | 129 | 183.733 | 185.426 | 28.198 | 1.00 17.77 | A | 0 |

| | | | | | | 37/73 | | | | |
|--------------|------------|----------|------------|---|------------|------------------------------------|------------------|--------------------------|--------|--------|
| ATOM | 64 | N | LEU | A | 130 | 185.618 186.620 | 27.979 | 1.00 16.79 | A | N |
| MOTA | 65 | CA | LEU | | | 186.479 185.540 | 28.425 | 1.00 19.53 | A | C |
| MOTA | 66 | CB | LEU | | | 187.943 186.006 | 28.392 | 1.00 19.86 | A | C |
| MOTA | 67 | CG | LEU | | | 189.050 184.967 | 28.619 | 1.00 22.85 | A | C |
| ATOM | 68 | - | LEU | | | 188.897 183.839 | 27.604 | 1.00 17.77 | A | C |
| ATOM | 69 70 | | LEU LEU | | | 190.429 185.631 186.090 185.081 | 28.492 29.834 | 1.00 16.04 1.00 21.19 | A A | C |
| MOTA MOTA | 70 71 | С О | LEU | | | 186.080 183.885 | 30.121 | 1.00 24.25 | A | Ö |
| MOTA | 72 | N | GLU | | | 185.756 186.032 | 30.705 | 1.00 23.78 | A | N |
| ATOM | 73 | CA | GLU | | | 185.349 185.729 | 32.082 | 1.00 25.83 | A | С |
| MOTA | 74 | CB | GLU | Α | 131 | 184.952 187.016 | 32.834 | 1.00 30.42 | A | C |
| MOTA | 75 | CG | GLU | | | 186.005 188.110 | 32.945 | 1.00 42.06 | A | С |
| MOTA | 76 | CD | GLU | | | 186.135 188.977 | 31.686 | 1.00 46.89 | A | C |
| MOTA | 77 | | GLU | | | 185.319 188.822 187.058 189.821 | 30.747 31.640 | 1.00 51.89 1.00 50.51 | A A | 0 |
| ATOM ATOM | 78 79 | C | GLU GLU | | | 184.146 184.751 | 32.145 | 1.00 30.31 | A | c |
| ATOM | 80 | Ö | GLU | | | 183.790 184.281 | 33.227 | 1.00 21.67 | A | ŏ |
| ATOM | 81 | N | ASP | | | 183.503 184.473 | 31.008 | 1.00 22.51 | A | N |
| MOTA | 82 | CA | ASP | A | 132 | 182.364 183.565 | 30.989 | 1.00 22.54 | A | С |
| ATOM | 83 | CB | ASP | | | 181.458 183.825 | | 1.00 24.79 | A | C |
| MOTA | 84 | CG | ASP | | | 180.631 185.120 | | 1.00 28.99 | A | C |
| ATOM | 85 | | ASP | | | 180.136 185.417 180.450 185.824 | | 1.00 29.67 1.00 26.45 | A A | 0 |
| ATOM ATOM | 86 87 | C | ASP ASP | | | 182.752 182.087 | | 1.00 28.45 | A | C |
| ATOM | 88 | 0 | ASP | | | 181.925 181.226 | | 1.00 22.12 | A | ŏ |
| ATOM | 89 | N | PHE | | 133 | 183.998 181.781 | | 1.00 23.02 | A | N |
| MOTA | 90 | CA | PHE | A | 133 | 184.411 180.378 | 30.554 | 1.00 22.89 | Α | C |
| ATOM | 91 | CB | PHE | | 133 | 184.812 179.998 | | 1.00 18.64 | A | C |
| ATOM | 92 | CG | PHE | | 133 | 183.901 180.565 | | 1.00 17.41 | A | C |
| ATOM | 93 94 | | PHE | | 133 | 184.042 181.884 182.904 179.783 | | 1.00 15.80 1.00 16.46 | A A | C C |
| ATOM ATOM | 95 | | PHE | | 133 | 183.215 182.414 | | 1.00 10.46 | A | c |
| ATOM | 96 | | PHE | | 133 | 182.063 180.305 | | 1.00 15.10 | A | č |
| MOTA | 97 | CZ | PHE | | 133 | 182.224 181.626 | 26.060 | 1.00 18.42 | Α | С |
| ATOM | 98 | С | PHE | | 133 | 185.557 179.984 | | 1.00 22.91 | A | С |
| ATOM | 99 | 0 | PHE | | 133 | 186.466 180.766 | | 1.00 24.66 | A | 0 |
| ATOM | 100 | N | GLU | | 134 134 | 185.484 178.767 186.566 178.248 | | 1.00 22.49 1.00 21.74 | A A | N |
| ATOM ATOM | 101 102 | CA CB | GLU | | 134 | 186.054 177.264 | | 1.00 21.74 | A | C |
| ATOM | 103 | CG | GLU | | 134 | 185.401 177.912 | | 1.00 29.62 | A | c |
| ATOM | 104 | CD | GLƯ | | 134 | 184.751 176.887 | | 1.00 37.53 | Α | С |
| ATOM | 105 | | GLU | | 134 | 185.460 175.983 | | 1.00 38.84 | Α | 0 |
| ATOM | 106 | | GLU | | 134 | 183.517 176.974 | | 1.00 43.58 | A | 0 |
| ATOM | 107 | С 0 | GLU GLU | | 134 134 | 187.313 177.528 186.702 176.784 | | 1.00 21.49 1.00 23.43 | A A | C |
| ATOM ATOM | 108 109 | Ŋ | ILE | | 135 | 188.608 177.794 | | 1.00 23.43 | A | И |
| ATOM | 110 | CA | ILE | | 135 | 189.425 177.197 | | 1.00 19.08 | A | c |
| ATOM | 111 | CB | ILE | | 135 | 190.554 178.149 | | 1.00 22.58 | A | C |
| MOTA | 112 | | ILE | | 135 | 191.285 177.543 | | 1.00 19.44 | A | С |
| ATOM | 113 | | ILE | | 135 | 189.990 179.541 | | 1.00 20.52 | A | C |
| ATOM | 114 | | ILE | | 135 135 | 188.876 179.535 190.099 175.941 | | 1.00 21.85 1.00 20.74 | A | C |
| ATOM ATOM | 115 116 | С 0 | ILE | | 135 | 190.667 175.944 | | 1.00 20.74 | A A | C |
| ATOM | 117 | N | | | 136 | 190.058 174.876 | | 1.00 19.98 | A | И |
| ATOM | 118 | CA | | | 136 | 190.688 173.629 | | 1.00 19.38 | A | C |
| MOTA | 119 | С | | | 136 | 191.995 173.397 | | 1.00 18.61 | A | С |
| ATOM | 120 | 0 | | | 136 | 192.742 174.324 | | 1.00 20.61 | A | 0 |
| ATOM | 121 | N | | | 137 | 192.267 172.156 | | 1.00 22.50 | A | N |
| ATOM ATOM | 122 123 | CA CB | | | 137 137 | 193.500 171.827 193.771 170.325 | | 1.00 22.75 1.00 22.49 | A A | C C |
| ATOM | 123 | CG | | | 137 | 192.820 169.474 | | 1.00 20.82 | A | C |
| ATOM | 125 | CD | | | 137 | 193.107 168.016 | | 1.00 15.70 | A | č |
| ATOM | 126 | NE | | | 137 | 192.212 167.104 | | 1.00 14.70 | A | N |
| MOTA | 127 | CZ | | | 137 | 192.299 166.784 | | 1.00 14.90 | A | С |
| ATOM | 128 | | ARG | | | 193.237 167.305 | | 1.00 13.75 | A | N |
| ATOM | 129 | | ARG | | | 191.462 165.900 193.396 172.183 | | 1.00 13.41 1.00 23.53 | A | N |
| ATOM ATOM | 130 131 | С 0 | | | 137 137 | 193.396 172.183 | | 1.00 23.53 | A A | С 0 |
| ATOM | 132 | И | | | 138 | 194.542 172.250 | | 1.00 22.98 | A | И |
| ATOM | 133 | CD | | | 138 | 195.850 172.477 | | 1.00 19.97 | A | C |
| | | | | | | | | | | |

| ATOM | 134 | CA | PRO A | A | 138 | 194.613 | 172.552 | 25.237 | 1.00 | 22.67 | A | С |
|--------------|------------|----------|------------|---|-----|--------------------|--------------------|------------------|------|----------------|--------|--------|
| ATOM | 135 | CB | PRO A | A | 138 | 196.116 | | 25.007 | 1.00 | | A | С |
| ATOM | 136 | CG | PRO A | | | 196.570 | | 26.295 | 1.00 | _ | A | C |
| MOTA | 137 | C | PRO I | | | 194.135 | | 24.497 | 1.00 | | A | C |
| ATOM | 138 | 0 | PRO I | | | 194.528 | | 24.876 | 1.00 | | A. | 0 |
| ATOM | 139 | N | LEU Z | | | 193.297 192.809 | | 23.471 22.716 | 1.00 | 19.70 | A A | N C |
| MOTA | 140 141 | CA CB | LEU A | | | 191.340 | | 22.718 | | 19.32 | A A | C |
| MOTA MOTA | 142 | CG | LEU | | | 190.349 | | 23.473 | | 18.46 | A | Ċ |
| ATOM | 143 | CD1 | LEU . | | | 188.966 | | 22.964 | | 16.26 | A | č |
| ATOM | 144 | CD2 | LEU . | | | 190.342 | | 24.163 | | 15.61 | A | С |
| MOTA | 145 | С | LEU . | A | 139 | 193.636 | 170.125 | 21.454 | 1.00 | 18.97 | A | C |
| MOTA | 146 | 0 | LEU . | Α | 139 | 193.714 | 169.045 | 20.883 | | 20.68 | A | 0 |
| ATOM | 147 | N | GLY . | | | 194.256 | | 21.026 | | 19.57 | A | N |
| ATOM | 148 | CA | GLY . | | | 195.056 | | 19.825 | | 16.45 | A | C |
| MOTA | 149 | C | GLY . | | | 195.821 | | 19.630 | | 18.41 | A | C |
| ATOM | 150 | 0 | GLY . | | | 195.560 196.778 | | 20.280 18.713 | | 17.66 23.54 | A A | N O |
| MOTA | 151 152 | N CA | LYS LYS | | | 197.635 | | 18.399 | | 25.64 | A | C |
| MOTA MOTA | 153 | CB | LYS | | | 199.103 | | 18.473 | | 29.50 | A | Ċ |
| ATOM | 154 | CG | LYS | | | 200.101 | | 18.080 | | 37.58 | A | C |
| MOTA | 155 | CD | LYS | | | 201.550 | | 18.187 | 1.00 | 42.29 | A | С |
| ATOM | 156 | CE | LYS | A | 141 | 202.483 | 174.918 | 17.891 | 1.00 | 46.12 | A | С |
| MOTA | 157 | ΝZ | LYS | | | 203.914 | | 17.890 | | 49.84 | A | N |
| MOTA | 158 | С | LYS | | | 197.313 | | 16.995 | | 26.94 | A | C |
| MOTA | 159 | 0 | LYS | | | 197.578 | | 15.986 | | 26.47 | A. | 0 |
| MOTA | 160 | И | GLY GLY | | | 196.724 196.392 | | 16.938 15.656 | | 26.51 26.65 | A A | N N |
| ATOM ATOM | 161 162 | CA C | GLY | | | 197.515 | | 15.234 | | 26.71 | A | C |
| ATOM | 163 | o | GLY | | | | 177.086 | 16.052 | | 26.93 | A | Ö |
| MOTA | 164 | N | LYS | | | 197.501 | | 13.969 | | 24.67 | A | N |
| ATOM | 165 | CA | LYS | | | 198.529 | 178.037 | 13.452 | 1.00 | 22.25 | A | С |
| ATOM | 166 | CB | LYS | A | 143 | | 178.220 | 11.925 | 1.00 | 25.89 | Α | C |
| MOTA | 167 | CG | LYS | | | 199.535 | | 11.307 | | 30.09 | A | C |
| MOTA | 168 | CD | LYS | | | | 179.060 | 9.792 | | 35.88 | A | C |
| ATOM | 169 | CE | LYS | | | | 180.037 | 9.330 | | 41.66 | A. | C |
| MOTA | 170 171 | NZ C | LYS LYS | | | 198.554 | 180.206 | 7.857 14.160 | | 42.97 | A A | N C |
| ATOM ATOM | 172 | Ö | LYS | | | | 179.921 | 14.425 | | 22.44 | A | Ö |
| ATOM | 173 | Ŋ | PHE | | | | 179.986 | 14.477 | | 20.35 | A | N |
| ATOM | 174 | CA | PHE | | | | 181.311 | 15.130 | 1.00 | 21.42 | A | С |
| MOTA | 175 | CB | PHE | A | 144 | | 182.258 | 14.362 | | 17.68 | Α | С |
| MOTA | 176 | CG | PHE | | | | 182.429 | 12.896 | | 22.16 | A | C |
| ATOM | 177 | | PHE | | | | 181.421 | 11.959 | | 20.33 | A | C |
| ATOM | 178 | | PHE | | | | 183.574 181.564 | 12.464 10.624 | | 23.47 20.91 | A. | C |
| ATOM ATOM | 179 180 | | PHE PHE | | | | 183.716 | 11.128 | | 21.10 | A A | C |
| ATOM | 181 | CZ | PHE | | | | 182.708 | 10.213 | | 18.55 | A | Č |
| MOTA | 182 | C | PHE | | | | 181.263 | 16.626 | | 20.47 | A | Ċ |
| ATOM | 183 | 0 | PHE | A | 144 | 196.668 | 182.283 | 17.246 | 1.00 | 20.98 | A | 0 |
| ATOM | 184 | N | GLY | | | | 180.072 | 17.208 | | 18.58 | A | N |
| ATOM | 185 | CA | | | 145 | | 179.915 | 18.616 | | 19.23 | A | C |
| MOTA | 186 | C | GLY | | | | 178.538 | 18.922 | | 20.99 | A | C |
| ATOM | 187 188 | O N | GLY ASN | | | | 177.756 178.233 | 18.016 20.204 | | 21.28 | A A | N O |
| ATOM ATOM | 189 | CA | ASN | | | | 176.938 | 20.598 | | 21.26 | A | C |
| ATOM | 190 | СВ | ASN | | | | 176.544 | 21.964 | | 24.59 | A | Ċ |
| ATOM | 191 | CG | ASN | | | | 176.352 | 21.939 | 1.00 | 27.16 | A | С |
| ATOM | 192 | OD1 | ASN | A | 146 | | 175.853 | 20.956 | | 32.36 | A | 0 |
| ATOM | 193 | | ASN | | | | 176.737 | 23.015 | | 27.51 | A | N |
| ATOM | 194 | С | | | 146 | | 176.878 | 20.683 | | 20.53 | A. | C |
| ATOM | 195 | O N | ASN | | | | 177.902 175.658 | 20.676 20.740 | | 20.90 | A A | O N |
| MOTA | 196 | N CA | VAL VAL | | | | 175.430 | 20.740 | | 14.64 | A | N C |
| MOTA ATOM | 197 198 | CB | | | 147 | | 174.515 | 19.799 | | 13.96 | A | . C |
| ATOM | 199 | | VAL | | | | 174.217 | 20.092 | | 10.05 | A | Ċ |
| ATOM | 200 | | VAL | | | 191.669 | 175.213 | 18.439 | 1.00 | 8.41 | A | C |
| ATOM | 201 | С | | | 147 | | 174.746 | 22.301 | | 16.21 | A | C |
| ATOM | 202 | 0 | | | 147 | | 173.783 | 22.523 | | 14.13 | A | 0 · |
| ATOM | 203 | N | TYR | A | 148 | 191.375 | 175.299 | 23.242 | 1.00 | 14.89 | A | N |
| | | | | | | | | | | | | |

| MOTA | 204 | CA | TYR | A | 148 | 191.315 | 174.786 | 24.614 | 1.00 | 14.47 | A | С |
|--------------|------------|-----------|------------|---|------------|---------|--------------------|------------------|------|----------------|--------|--------|
| ATOM | 205 | CB | TYR | | | | 175.891 | 25.642 | | 12.68 | A | С |
| MOTA | 206 | CG | TYR | | | | 176.619 | 25.491 | _ | 18.66 | A | C |
| MOTA | 207 | | TYR | | | | 177.690 | 24.605 | | 16.46 18.77 | A | C |
| ATOM ATOM | 208 209 | | TYR | | | | 178.347 176.222 | 24.434 26.217 | | 15.67 | A A | c |
| ATOM | 210 | | TYR | | | | 176.880 | 26.050 | | 20.14 | A | č |
| ATOM | 211 | CZ | TYR | | | | 177.938 | 25.153 | | 18.86 | A | Č |
| ATOM | 212 | OH | TYR | | | 196.555 | 178.569 | 24.934 | 1.00 | 23.63 | A | 0 |
| MOTA | 213 | С | TYR | | | | 174.234 | 24.936 | | 13.13 | A | С |
| MOTA | 214 | 0 | TYR | | | | 174.674 | 24.386 | | 14.07 | A | 0 |
| MOTA | 215 | N C7 | LEU | | | | 173.265 | 25.831 | | 11.62 | A A | N |
| ATOM ATOM | 216 217 | CA CB | LEU | | | | 172.753 171.466 | 26.223 27.003 | | 11.86 10.50 | A A | C C |
| ATOM | 218 | CG | LEU | | | | 170.675 | 27.388 | | 12.61 | A | Ċ |
| MOTA | 219 | CD1 | LEU | A | 149 | 186.695 | 170.364 | 26.182 | 1.00 | 11.20 | A | С |
| MOTA | 220 | CD2 | LEU | Α | 149 | 188.001 | 169.410 | 28.051 | | 11.24 | A | С |
| MOTA | 221 | C | LEU | | | | 173.911 | 27.101 | | 13.55 | A | C |
| MOTA | 222 | 0 | LEU | | | | 174.728 | 27.565 | | 12.48 14.24 | A | 0 |
| MOTA MOTA | 223 224 | N CA | ALA ALA | | | | 174.008 175.102 | 27.316 28.120 | | 15.20 | A A | N C |
| ATOM | 225 | CB | ALA | | | | 176.406 | 27.318 | | 15.60 | A | Č |
| ATOM | 226 | C | | | 150 | | 174.800 | 28.612 | | 17.25 | A | C |
| MOTA | 227 | 0 | ALA | A | 150 | | 173.929 | 28.083 | 1.00 | 18.30 | A | 0 |
| MOTA | 228 | N | ARG | | | | 175.532 | 29.629 | | 17.29 | A | N |
| MOTA | 229 230 | CA | ARG | | | | 175.334 174.479 | 30.215 31.492 | | 19.70 20.02 | A | C |
| MOTA MOTA | 231 | CB CG | | | 151 151 | | 174.102 | 32.258 | | 26.58 | A A | c |
| ATOM | 232 | CD | ARG | | | | 173.557 | 33.686 | | 30.64 | A | c |
| ATOM | 233 | NE | ARG | A | 151 | 183.235 | 172.405 | 33.673 | 1.00 | 32.15 | Α | N |
| MOTA | 234 | CZ | | | 151 | | 171.151 | 33.348 | | 33.18 | Α | С |
| ATOM | 235 | | ARG | | | | 170.851 | 33.004 | | 33.09 | A | N |
| ATOM | 236 237 | NH2 C | ARG | | | | 170.190 176.707 | 33.362 30.518 | | 31.48 | A | N |
| ATOM ATOM | 238 | o | | | 151 151 | | 177.560 | 31.163 | | 19.62 | A A | 0 |
| ATOM | 239 | N | | | 152 | | 176.939 | 30.006 | | 21.84 | A | N |
| MOTA | 240 | CA | GLU | Α | 152 | 180.633 | 178.196 | 30.264 | 1.00 | 21.85 | A | С |
| ATOM | 241 | CB | | | 152 | | 178.298 | 29.377 | | 26.06 | Α | C |
| ATOM | 242 | CG | | | 152 | | 179.690 180.078 | 29.289 | | 28.31 | A | C |
| ATOM ATOM | 243 244 | CD OE1 | GLU | | 152 152 | | 180.804 | 30.543 31.391 | | 32.60 33.50 | A A | С 0 |
| MOTA | 245 | | GLU | | | | 179.650 | 30.679 | | 29.24 | A | Ö |
| ATOM | 246 | С | | | 152 | 180.252 | 178.091 | 31.742 | | 21.10 | A | C |
| ATOM | 247 | 0 | | | 152 | | 177.102 | 32.172 | | 19.62 | Α | 0 |
| ATOM | 248 | N | | | 153 | | 179.114 | 32.504 | | 21.06 | A | И |
| ATOM ATOM | 249 250 | CA CB | | | 153 153 | | 179.156 180.417 | 33.933 34.513 | | 20.90 | A A | C C |
| ATOM | 251 | CG | | | 153 | | 180.458 | 34.440 | | 22.17 | A | C |
| ATOM | 252 | CD | | | 153 | | 181.720 | 35.091 | | 21.22 | A | Č |
| ATOM | 253 | CE | | | 153 | | 181.658 | 35.002 | | 22.77 | Α | С |
| ATOM | 254 | NZ | | | 153 | | 182.877 | 35.572 | | 24.11 | A | N |
| ATOM | 255 256 | 0 | | | 153 153 | | 179.048 178.362 | 34.421 35.390 | | 21.26 | A | C |
| ATOM ATOM | 257 | Ŋ | | | 154 | | 179.704 | 33.786 | | 25.58 23.03 | A A | O N |
| ATOM | 258 | CA | | | 154 | | 179.579 | 34.330 | | 23.96 | A | C |
| MOTA | 259 | CB | GLN | A | 154 | | 180.686 | 33.800 | | 23.79 | A | C |
| MOTA | 260 | CG | | | 154 | | 182.053 | 34.288 | | 24.55 | Α | С |
| ATOM | 261 | CD | | | 154 | | 183.133 | 33.709 | | 24.55 | A | C |
| ATOM ATOM | 262 263 | | GLN GLN | | | | 184.283 182.779 | 33.617 33.309 | | 23.87 22.50 | A A | O N |
| ATOM | 264 | C | | | 154 | | 178.229 | 34.086 | | 24.10 | A | C |
| ATOM | 265 | 0 | | | 154 | | 177.675 | 34.996 | | 25.34 | A | ō |
| ATOM | 266 | N | | | 155 | | 177.700 | 32.871 | 1.00 | 22.36 | A | N |
| ATOM | 267 | CA | | | 155 | | 176.441 | 32.585 | | 21.24 | A | C |
| ATOM | 268 | CB | | | 155 | | 176.517 | 31.180 | | 20.38 | A | C |
| ATOM ATOM | 269 270 | OG C | | | 155 155 | | 176.607 175.182 | 30.282 32.691 | | 22.24 23.66 | A A | 0 |
| MOTA | 271 | õ | | | 155 | | 174.048 | 32.677 | | 20.04 | A | o |
| ATOM | 272 | N | | | 156 | | 175.406 | 32.789 | | 23.61 | A | N |
| ATOM | 273 | CA | LYS | A | 156 | 178.572 | 174.358 | 32.849 | 1.00 | 24.47 | A | С |
| | | | | | | | | | | | | |

| MOTA | 274 | CB | LYS | A | 156 | 178.350 | 173.467 | 34.065 | 1.00 | 25.24 | A. | С |
|------|-----|-----|-----|---|------------|---------|---------|--------|------|-------|----|--------|
| ATOM | 275 | CG | LYS | Α | 156 | 178.523 | 174.254 | 35.368 | 1.00 | 32.64 | A | С |
| ATOM | 276 | CD | LYS | Α | 156 | 178.309 | 173.358 | 36.552 | 1.00 | 35.73 | A | С |
| ATOM | 277 | CE | | | 156 | 178.506 | | 37.870 | 1.00 | | A. | c |
| MOTA | 278 | NZ | | | 156 | 178.457 | | 38.978 | | 42.75 | A | N |
| | 279 | C | | | 156 | 178.634 | | 31.548 | 1.00 | | | c |
| ATOM | | | | | | | | | | | A. | |
| MOTA | 280 | 0 | LYS | | | 179.131 | _ | 31.509 | 1.00 | | A. | 0 |
| MOTA | 281 | N | PHE | | 157 | 178.152 | | 30.472 | | 20.94 | A | N |
| ATOM | 282 | CA | PHE | Α | 157 | 178.180 | 173.530 | 29.162 | 1.00 | 19.88 | A. | С |
| ATOM | 283 | CB | PHE | A | 157 | 177.370 | 174.367 | 28.174 | 1.00 | 21.87 | A | C |
| ATOM | 284 | CG | PHE | A | 157 | 177.209 | 173.735 | 26.840 | 1.00 | 22.62 | A | С |
| MOTA | 285 | CD1 | PHE | A | 157 | 176.501 | 172.546 | 26.704 | 1.00 | 26.84 | A. | С |
| MOTA | 286 | CD2 | PHE | Α | 157 | 177.745 | 174.336 | 25.707 | 1.00 | 24.18 | A | С |
| ATOM | 287 | CE1 | PHE | А | 157 | 176.326 | 171.957 | 25.448 | 1.00 | 27.13 | A | С |
| ATOM | 288 | | PHE | | 157 | 177.576 | | 24.446 | | 24.84 | A | C |
| MOTA | 289 | CZ | PHE | | 157 | | 172.574 | 24.316 | | 26.19 | A | Ċ |
| ATOM | 290 | C | | | 157 | 179.645 | | 28.708 | | 20.86 | A | č |
| | | | PHE | | | | 174.451 | 28.739 | | | | |
| ATOM | 291 | 0 | | | 157 | | | | | 16.68 | A. | 0 |
| ATOM | 292 | N | | | 158 | | 172.243 | 28.316 | | 18.62 | A | N |
| MOTA | 293 | CA | ILE | | 158 | | 171.997 | 27.862 | | 17.65 | A | С |
| ATOM | 294 | CB | | | 158 | | 170.521 | 28.156 | | 21.22 | A | С |
| ATOM | 295 | | | | 158 | | 170.183 | 27.472 | | 20.54 | A | С |
| ATOM | 296 | CG1 | ILE | A | 158 | 181.998 | 170.339 | 29.675 | 1.00 | 25.44 | A | С |
| ATOM | 297 | CD1 | ILE | Α | 158 | 181.751 | 168.898 | 30.193 | 1.00 | 32.22 | A | С |
| ATOM | 298 | С | ILE | Α | 158 | 181.502 | 172.306 | 26.363 | 1.00 | 19.32 | A | С |
| ATOM | 299 | 0 | ILE | A | 158 | 180.622 | 171.940 | 25.588 | 1.00 | 21.25 | A | 0 |
| MOTA | 300 | N | LEU | A | 159 | 182.544 | 173.021 | 25.958 | | 19.68 | A | N |
| ATOM | 301 | CA | | | 159 | | 173.365 | 24.552 | | 18.03 | A | C |
| ATOM | 302 | CB | | | 159 | | 174.625 | 24.214 | | 18.70 | A | Č |
| ATOM | 303 | CG | | | 159 | | 175.726 | 25.275 | | 18.81 | A | c |
| MOTA | 304 | | LEU | | | | 176.522 | 25.197 | | 25.89 | A. | C |
| | | | LEU | | | | 176.522 | | | | | |
| ATOM | 305 | | | | | | | 25.065 | | 15.33 | A. | C |
| ATOM | 306 | C | | | 159 | | 173.553 | 24.263 | | 16.64 | A. | C |
| ATOM | 307 | 0 | | | 159 | | 173.211 | 25.099 | | 10.64 | A | 0 |
| MOTA | 308 | N | | | 160 | | 174.069 | 23.084 | | 14.09 | A | N |
| ATOM | 309 | CA | | | 160 | | 174.271 | 22.742 | | 14.90 | A | C |
| ATOM | 310 | CB | | | 160 | 186.371 | 173.394 | 21.574 | 1.00 | 11.94 | A | C |
| MOTA | 311 | С | ALA | A | 160 | 186.230 | 175.736 | 22.420 | 1.00 | 15.35 | A | С |
| ATOM | 312 | 0 | ALA | A | 160 | 185.419 | 176.377 | 21.777 | 1.00 | 16.22 | A | 0 |
| ATOM | 313 | N | LEU | A | 161 | 187.348 | 176.277 | 22.876 | 1.00 | 17.51 | A | N |
| ATOM | 314 | CA | LEU | A | 161 | 187.656 | 177.685 | 22.636 | 1.00 | 17.81 | A | С |
| MOTA | 315 | CB | LEU | A | 161 | 187.959 | 178.379 | 23.958 | 1.00 | 19.09 | A | С |
| ATOM | 316 | CG | LEU | A | 161 | 187.661 | 179.882 | 24.003 | | 24.28 | A | C |
| ATOM | 317 | | LEU | | | | 180.085 | 23.715 | | 19.74 | A | Č |
| ATOM | 318 | | LEU | | | | 180.482 | 25.396 | | 26.64 | A | Č |
| MOTA | 319 | C | | | 161 | | 177.829 | 21.697 | | 18.94 | A | C |
| ATOM | 320 | ŏ | | | 161 | | 177.506 | | | 15.15 | A | |
| | | | | | | | 178.300 | | | | | 0 |
| ATOM | 321 | N | | | 162 162 | | | 20.477 | | 15.44 | A. | N |
| ATOM | 322 | CA | | | | | 178.489 | 19.506 | | 16.27 | A | C |
| ATOM | 323 | CB | | | 162 | | 178.254 | 18.093 | | 15.06 | A | C |
| ATOM | 324 | CG | | | 162 | | 178.338 | 17.036 | | 13.12 | A | С |
| ATOM | 325 | CD | | | 162 | | 177.968 | 15.682 | | 15.23 | A | С |
| MOTA | 326 | CE | | | 162 | | 178.025 | 14.590 | | 15.94 | A | С |
| ATOM | 327 | NZ | | | 162 | | 177.625 | 13.262 | 1.00 | 21.75 | A | N |
| MOTA | 328 | С | | | 162 | 190.220 | 179.909 | 19.626 | 1.00 | 16.04 | A | С |
| MOTA | 329 | 0 | LYS | Α | 162 | 189.486 | 180.863 | 19.427 | 1.00 | 17.16 | A | 0 |
| MOTA | 330 | N | VAL | Α | 163 | 191.501 | 180.044 | 19.955 | 1.00 | 15.21 | A | N |
| ATOM | 331 | CA | VAL | A | 163 | 192.110 | 181.357 | 20.107 | 1.00 | 16.50 | A | С |
| ATOM | 332 | CB | VAL | Α | 163 | 193.047 | 181.400 | 21.336 | 1.00 | 17.79 | A | С |
| ATOM | 333 | | VAL | Α | 163 | | 182.816 | 21.546 | | 15.20 | A | C |
| ATOM | 334 | | | | 163 | | 180.897 | 22.578 | | 14.92 | A. | Č |
| ATOM | 335 | c | | | 163 | | 181.758 | 18.888 | | 17.82 | A | c |
| ATOM | 336 | Ö | | | 163 | | 180.933 | 18.287 | | | | |
| | 337 | | | | 164 | | 183.028 | | | 20.09 | A. | O N |
| MOTA | | N | | | | | | 18.522 | | 18.13 | A | N |
| ATOM | 338 | CA | | | 164 | | 183.509 | 17.387 | | 15.87 | A. | C |
| MOTA | 339 | CB | | | 164 | | 183.802 | 16.203 | | 18.86 | A. | С |
| ATOM | 340 | CG | | | 164 | | 182.603 | 15.752 | | 20.75 | A. | С |
| MOTA | 341 | | | | 164 | | 182.980 | 15.575 | | 23.26 | A | С |
| ATOM | 342 | | | | 164 | | 182.084 | 14.477 | | 19.09 | A. | С |
| MOTA | 343 | C | LEU | Α | 164 | 194.352 | 184.789 | 17.835 | 1.00 | 16.04 | A | С |
| | | | | | | | | | | | | |

| ATOM | 344 | 0 | LEU | Α | 164 | 193.687 | 185.709 | 18.295 | 1.00 | 13.41 | A | 0 |
|------|-----|-----|-----|---|-----|----------|---------|--------|------|-------|---|-----|
| ATOM | 345 | N | PHE | | | | 184.858 | 17.738 | | 15.52 | A | N |
| ATOM | 346 | CA | PHE | | | 196.340 | | 18.141 | | 18.33 | A | _ |
| | | | | | | 197.804 | | | | | | |
| ATOM | 347 | CB | PHE | | | | | 18.497 | | 19.71 | A | |
| ATOM | 348 | CG | PHE | | | | 185.214 | 19.850 | | 26.23 | A | |
| ATOM | 349 | CD1 | PHE | Α | 165 | 197.826 | 183.840 | 20.033 | 1.00 | 27.06 | A | С |
| ATOM | 350 | CD2 | PHE | Α | 165 | 198.222 | 186.025 | 20.961 | 1.00 | 28.47 | A | C |
| MOTA | 351 | | PHE | | | | 183.281 | 21.298 | | 32.07 | A | С |
| | 352 | | PHE | | | | 185.479 | 22.239 | | | A | |
| ATOM | | | | | | | | | | 31.56 | | |
| ATOM | 353 | CZ | PHE | | | | 184.104 | 22.411 | | 35.02 | A | |
| ATOM | 354 | С | PHE | Α | 165 | 196.228 | 187.062 | 16.989 | 1.00 | 19.49 | A | C |
| MOTA | 355 | 0 | PHE | Α | 165 | 196.610 | 186.742 | 15.857 | 1.00 | 21.60 | A | 0 |
| ATOM | 356 | N | LYS | | | | 188.242 | 17.277 | | 18.17 | A | |
| | 357 | CA | LYS | | | | 189.299 | 16.282 | | 17.63 | A | |
| ATOM | | | | | | | | | | | | |
| ATOM | 358 | CB | LYS | | | | 190.520 | 16.931 | | 16.68 | A | |
| MOTA | 359 | CG | LYS | | | 193.319 | 190.346 | 17.376 | 1.00 | 15.54 | A | |
| ATOM | 360 | CD | LYS | Α | 166 | 192.703 | 191.672 | 17.826 | 1.00 | 10.39 | A | С |
| ATOM | 361 | CE | LYS | Α | 166 | 191.259 | 191.452 | 18.272 | 1.00 | 12.43 | A | С |
| ATOM | 362 | NZ | LYS | | | 190.505 | 192.644 | 18.792 | 1.00 | 7.46 | A | N |
| | 363 | C | | | 166 | | 189.792 | 15.536 | | 19.44 | A | |
| MOTA | | | | | | | | | | | | |
| ATOM | 364 | 0 | LYS | | | | 190.103 | 14.343 | | 19.53 | A | |
| ATOM | 365 | N | ALA | Α | 167 | | 189.885 | 16.237 | 1.00 | 19.10 | A | N |
| MOTA | 366 | CA | ALA | Α | 167 | 199.068 | 190.369 | 15.628 | 1.00 | 18.82 | A | С |
| ATOM | 367 | CB | ALA | Α | 167 | 200.140 | 190.591 | 16.710 | 1.00 | 11.48 | A | С |
| MOTA | 368 | C | | | 167 | | 189.377 | 14.571 | | 18.71 | A | |
| | 369 | Ö | | | 167 | | 189.762 | 13.534 | | 19.61 | A | |
| ATOM | | | | | | | | | | | | |
| MOTA | 370 | N | | | 168 | | 188.092 | 14.840 | | 18.71 | A | |
| MOTA | 371 | CA | | | 168 | | 187.039 | 13.907 | | 18.86 | A | |
| ATOM | 372 | CB | GLN | Α | 168 | 199.584 | 185.666 | 14.561 | 1.00 | 21.65 | A | C |
| ATOM | 373 | CG | GLN | Α | 168 | 200.584 | 184.664 | 14.014 | 1.00 | 25.64 | A | C |
| MOTA | 374 | CD | GUN | A | 168 | 200.544 | 183.310 | 14.690 | 1.00 | 29.19 | A | |
| | 375 | | GLN | | | | 183.208 | 15.900 | | 27.17 | A | |
| ATOM | | | | | | | | | | | | |
| ATOM | 376 | | GLN | | | | 182.249 | 13.920 | | 28.74 | A | |
| MOTA | 377 | С | GLN | A | 168 | 198.824 | 187.137 | 12.688 | 1.00 | 17.82 | A | . C |
| ATOM | 378 | 0 | GLN | Α | 168 | 199.273 | 187.079 | 11.560 | 1.00 | 20.56 | A | . 0 |
| ATOM | 379 | N | LEU | Α | 169 | 197.530 | 187.289 | 12.931 | 1.00 | 19.46 | A | N |
| ATOM | 380 | CA | | | 169 | | 187.404 | 11.848 | | 19.86 | A | |
| MOTA | 381 | СВ | | | 169 | | 187.572 | 12.393 | | 20.65 | A | |
| | | | | | | | | | | | | |
| MOTA | 382 | CG | | | 169 | | 186.370 | 13.052 | | 24.58 | Α | |
| ATOM | 383 | | LEU | | | | 186.837 | 13.566 | | 23.53 | A | C |
| ATOM | 384 | CD2 | LEU | Α | 169 | 194.396 | 185.189 | 12.069 | 1.00 | 20.67 | A | C |
| MOTA | 385 | С | LEU | Α | 169 | 196.802 | 188.604 | 10.961 | 1.00 | 21.12 | A | С |
| ATOM | 386 | 0 | LEU | Α | 169 | 196.533 | 188.564 | 9.761 | 1.00 | 17.39 | Α | . 0 |
| ATOM | 387 | N | | | 170 | | 189.697 | 11.564 | | 22.51 | A | |
| | | | | | 170 | | 190.915 | | | | | |
| ATOM | 388 | CA | - | | | | | 10.807 | | 23.02 | A | |
| ATOM | 389 | CB | | | 170 | | 192.102 | 11.769 | | 22.68 | A | |
| ATOM | 390 | CG | GLU | Α | 170 | | 192.607 | 12.232 | 1.00 | 27.99 | A | . с |
| ATOM | 391 | CD | GLU | Α | 170 | 196.294 | 193.330 | 13.579 | 1.00 | 31.84 | A | С |
| MOTA | 392 | OE1 | GLU | Α | 170 | 197.334 | 193.955 | 13.920 | 1.00 | 33.33 | Α | 0 |
| ATOM | 393 | | GLU | | | | 193.278 | 14.285 | 1.00 | 31.22 | A | |
| ATOM | 394 | C | | | 170 | | 190.753 | 9.949 | | 21.03 | A | |
| | | | | | | | | | | | | |
| MOTA | 395 | 0 | | | 170 | | 191.068 | 8.757 | | 23.09 | A | |
| MOTA | 396 | N | | | 171 | | 190.220 | 10.535 | | 17.25 | A | |
| ATOM | 397 | CA | LYS | Α | 171 | 201.059 | 190.014 | 9.790 | 1.00 | 19.63 | A | . С |
| ATOM | 398 | CB | LYS | Α | 171 | 202.139 | 189.442 | 10.706 | 1.00 | 21.18 | A | С |
| ATOM | 399 | CG | | | 171 | 203.525 | 189.395 | 10.073 | 1.00 | 25.15 | A | |
| MOTA | 400 | CD | | | 171 | | 188.888 | 11.054 | | 28.24 | A | |
| | | | | | | | | 10.395 | | | | |
| ATOM | 401 | CE | | | 171 | | 188.807 | | | 32.60 | A | _ |
| ATOM | 402 | NZ | | | 171 | | 188.297 | 11.331 | | 33.23 | A | |
| MOTA | 403 | С | LYS | Ą | 171 | 200.838 | 189.074 | 8.609 | 1.00 | 19.42 | A | С |
| ATOM | 404 | 0 | LYS | Α | 171 | 201.451 | 189.235 | 7.551 | 1.00 | 21.92 | A | 0 |
| ATOM | 405 | N | | | 172 | 199.957 | 188.095 | 8.782 | 1.00 | 17.92 | A | |
| ATOM | 406 | CA | | | 172 | | 187.126 | 7.720 | | 18.61 | A | |
| | | | | | | | | | | | | |
| ATOM | 407 | CB | | | 172 | | 185.826 | 8.341 | | 13.39 | A | |
| ATOM | 408 | С | | | 172 | | 187.627 | 6.679 | | 16.48 | A | |
| ATOM | 409 | 0 | ALA | Α | 172 | | 187.082 | 5.577 | 1.00 | 18.45 | A | 0 |
| ATOM | 410 | N | GLY | A | 173 | 197.890 | 188.651 | 7.053 | 1.00 | 16.48 | A | N |
| MOTA | 411 | CA | | | 173 | | 189.241 | 6.178 | | 17.37 | A | |
| | 412 | C | | | 173 | | 188.297 | 5.904 | | 18.48 | A | |
| ATOM | | | | | | | | | | | | |
| ATOM | 413 | 0 | GГХ | A | 173 | TAD. TOR | 188.264 | 4.789 | 1.00 | 17.50 | A | 0 |
| | | | | | | | | | | | | |

| ATOM | 414 | N | VAL. | Δ | 174 | 195.34 | 4 187.536 | 6.921 | 1.00 16.39 | A | N |
|------|-----|-----|------|---|-----|---------|--------------------|--------|------------|---|---|
| ATOM | 415 | CA | | | 174 | | 4 186.573 | | | | |
| | | | | | | | | | 1.00 18.80 | | C |
| ATOM | 416 | CB | | | 174 | | 8 185.171 | | 1.00 17.75 | | С |
| MOTA | 417 | | JAV | | | | 6 184 <i>.</i> 770 | | 1.00 17.03 | A | С |
| ATOM | 418 | CG2 | VAL | A | 174 | 195.16 | 6 185.207 | 8.684 | 1.00 12.69 | Α | С |
| ATOM | 419 | С | VAL | A | 174 | 193.01 | 5 186.982 | 7.535 | 1.00 19.69 | A | С |
| ATOM | 420 | 0 | | | 174 | | 2 186.152 | | 1.00 22.14 | | Ö |
| ATOM | 421 | N | | | 175 | | 0 188.282 | | | | |
| | | | | | | | | | 1.00 24.29 | | N |
| ATOM | 422 | CA | | | 175 | | 1 188.834 | | 1.00 25.76 | | С |
| MOTA | 423 | CB | GLU | A | 175 | | 2 190.351 | | 1.00 29.22 | A | С |
| MOTA | 424 | CG | GLU | Α | 175 | 193.33 | 3 190.938 | 8.903 | 1.00 38,41 | Α | С |
| MOTA | 425 | CD | GLU | Α | 175 | 193.99 | 8 191.112 | 7.548 | 1.00 39.97 | A | С |
| ATOM | 426 | OE1 | GLU | | | | 0 190.986 | | 1.00 47.49 | | ŏ |
| ATOM | 427 | | GLU | | | | 6 191.382 | | | | |
| | | | | | | | | | 1.00 46.22 | | 0 |
| MOTA | 428 | С | | | 175 | | 2 188.611 | | 1.00 25.95 | | C |
| ATOM | 429 | 0 | GLU | A | 175 | | 3 188.313 | | 1.00 25.42 | A | 0 |
| MOTA | 430 | N | HIS | Α | 176 | 190.48 | 3 188.768 | 6.438 | 1.00 26.45 | A | N |
| ATOM | 431 | CA | HIS | Α | 176 | 189.25 | 4 188.539 | 5.708 | 1.00 24.68 | А | С |
| MOTA | 432 | CB | | | 176 | | 6 189.074 | | 1.00 23.09 | | Ċ |
| ATOM | 433 | CG | | | 176 | | 3 189.014 | | | | |
| | | | | | | | | | 1.00 32.41 | | C |
| ATOM | 434 | | HIS | | | | 0 188.363 | | 1.00 34.18 | | С |
| ATOM | 435 | | HIS | | | | 5 189.576 | | 1.00 32.75 | A | N |
| ATOM | 436 | | | | 176 | 185.79 | 6 189.266 | 3.406 | 1.00 33.74 | A | С |
| ATOM | 437 | NE2 | HIS | A | 176 | 186.20 | 7 188.529 | 2.386 | 1.00 34.72 | A | N |
| ATOM | 438 | С | | | 176 | | 8 187.062 | | 1.00 23.32 | | Ċ |
| MOTA | 439 | Ö | | | 176 | | 1 186.755 | | 1.00 23.52 | | o |
| | | | | | | | | | | | |
| ATOM | 440 | N | | | 177 | | 3 186.137 | | 1.00 21.78 | | N |
| ATOM | 441 | CA | | | 177 | | 2 184.721 | | 1.00 19.85 | | С |
| ATOM | 442 | CB | | | 177 | | 8 183.818 | | 1.00 21.23 | A | С |
| MOTA | 443 | CG | GLN | Α | 177 | 191.17 | 3 183.994 | 3.977 | 1.00 23.08 | A | С |
| ATOM | 444 | CD | GLN | A | 177 | 192.11 | 3 185.179 | 3.856 | 1.00 26.14 | A | С |
| ATOM | 445 | OE1 | GLN | | | | 1 186.204 | | 1.00 27.02 | A | ō |
| ATOM | 446 | | GLN | | | | 1 185.056 | | 1.00 27.02 | | |
| | | | | | | | | | | | N |
| ATOM | 447 | С | | | 177 | | 9 184.317 | | 1.00 18.66 | | С |
| ATOM | 448 | 0 | | | 177 | 188.05 | | | 1.00 18.16 | A | 0 |
| ATOM | 449 | N | LEU | Α | 178 | 189.26 | 7 185.001 | 8.202 | 1.00 17.80 | A | N |
| MOTA | 450 | CA | LEU | Α | 178 | 188.74 | 2 184.695 | 9.532 | 1.00 17.25 | A | С |
| ATOM | 451 | CB | LEU | A | 178 | 189.47 | 3 185.495 | 10.616 | 1.00 14.48 | A | С |
| MOTA | 452 | CG | LEU | А | 178 | | 8 185.297 | | 1.00 14.78 | A | č |
| ATOM | 453 | | LEU | | | | 2 183.792 | _ | 1.00 13.65 | | |
| ATOM | 454 | | LEU | | | | | | | A | C |
| | | | | | | | 4 185.964 | | 1.00 15.52 | A | С |
| ATOM | 455 | C | | | 178 | 187.25 | | | 1.00 18.82 | A | C |
| ATOM | 456 | 0 | | | 178 | 186.43 | 6 184.346 | 10.148 | 1.00 18.56 | A | 0 |
| ATOM | 457 | N | ARG | A | 179 | 186.92 | 9 186.171 | 8.950 | 1.00 17.14 | A | N |
| MOTA | 458 | CA | ARG | A | 179 | 185.57 | 0 186.637 | 8.893 | 1.00 20.36 | A | C |
| ATOM | 459 | CB | ARG | Α | 179 | 185.54 | 7 188.004 | 8.238 | 1.00 24.60 | A | č |
| ATOM | 460 | CG | | | 179 | | 1 188.581 | | | | |
| MOTA | 461 | CD | | | 179 | | 9 189.355 | 8.190 | 1.00 30.51 | A | C |
| | | | | | | | | 6.937 | 1.00 34.92 | A | C |
| ATOM | 462 | NE | | | 179 | | 2 190.700 | | 1.00 44.42 | A | N |
| MOTA | 463 | CZ | | | 179 | | 8 191.679 | 7.721 | 1.00 50.64 | A | С |
| ATOM | 464 | | ARG | | | 185.60 | 9 191.475 | 8.060 | 1.00 53.62 | A | N |
| MOTA | 465 | NH2 | ARG | Α | 179 | 183.80 | 0 192.881 | 7.910 | 1.00 54.27 | A | N |
| ATOM | 466 | С | ARG | Α | 179 | 184.67 | 7 185.663 | 8.112 | 1.00 20.68 | A | C |
| ATOM | 467 | 0 | | | 179 | | 6 185.428 | 8.490 | 1.00 20.49 | A | ő |
| ATOM | 468 | N | | | 180 | | 1 185.102 | 7.027 | 1.00 16.87 | | |
| | 469 | CA | | | | | | | | A | N |
| ATOM | | | | | 180 | | 7 184.139 | 6.240 | 1.00 16.27 | A | C |
| ATOM | 470 | CB | ARG | | | | 5 183.851 | 4.880 | 1.00 15.64 | A | C |
| MOTA | 471 | CG | | | 180 | 185.03 | 5 184.997 | 3.869 | 1.00 19.03 | A | С |
| MOTA | 472 | CD | ARG | Α | 180 | 185.243 | 3 184.593 | 2.394 | 1.00 19.17 | A | С |
| ATOM | 473 | NE | ARG | Α | 180 | 186.53 | 6 183.973 | 2.158 | 1.00 22.25 | A | N |
| ATOM | 474 | CZ | ARG | | | | 3 184.003 | 1.011 | 1.00 22.42 | A | C |
| ATOM | 475 | | ARG | | | | 3 184.633 | -0.067 | 1.00 16.67 | | |
| | | | | | | | | | | A | N |
| ATOM | 476 | | ARG | | | | 183.384 | 0.949 | 1.00 23.03 | A | N |
| ATOM | 477 | C | ARG | | | | 182.837 | 7.037 | 1.00 16.14 | A | С |
| ATOM | 478 | 0 | ARG | | | | 5 182.207 | 6.950 | 1.00 17.78 | A | 0 |
| MOTA | 479 | N | GLU | Α | 181 | 185.294 | 1 182.439 | 7.812 | 1.00 15.13 | A | N |
| MOTA | 480 | CA | GLU | | | 185.211 | 181.222 | 8.627 | 1.00 15.82 | A | c |
| ATOM | 481 | СВ | GLU | | | | 180.969 | 9.431 | 1.00 17.60 | A | Č |
| ATOM | 482 | CG | GLU | | | | 7 179.610 | 10.164 | 1.00 17.00 | A | c |
| ATOM | | CD | | | | | 7 179.010 | | | | |
| MION | 483 | CD | GLU | A | TOT | 10/.// | , 1,3.633 | 11.023 | 1.00 29.50 | A | С |
| | | | | | | | | | | | |

| AROM 486 OEZ GLU A 181 188.877 179.898 10.811 1.00 23.91 A O AROM 486 C GLU A 181 194.059 181.374 9.615 1.00 17.24 A C AROM 487 O GLU A 181 194.059 181.374 9.615 1.00 17.24 A C AROM 487 O GLU A 181 194.075 182.486 10.336 1.00 16.10 A A N AROM 489 C VAL A 182 184.075 182.486 10.336 1.00 16.10 A A N AROM 489 C VAL A 182 184.075 182.486 10.336 1.00 16.10 A A N AROM 489 C VAL A 182 184.075 182.486 10.336 1.00 16.10 A A N AROM 490 CB VAL A 182 184.075 182.486 10.336 1.00 16.10 A A C AROM 490 CB VAL A 182 184.075 182.486 10.336 1.00 16.10 A A C AROM 491 CB VAL A 182 184.675 183.769 12.946 1.00 15.96 A C AROM 491 CB VAL A 182 184.675 183.769 12.946 1.00 15.96 A C AROM 494 C VAL A 182 184.675 183.769 12.946 1.00 15.96 A C AROM 494 C VAL A 182 184.675 183.810 190.755 1.00 16.14 A C AROM 495 N GLU A 183 181.491 183.805 9.788 1.00 16.54 A N AROM 496 CA GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 499 CD GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 499 CD GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.477 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.474 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.974 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.474 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.474 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.934 A C AROM 500 CB GLU A 183 180.566 187.674 7.874 1.00 24.054 A AROM 500 | | | | | | | | | | | | | | |
|--|------|-----|-----|-------|---|-----|---|---------|---------|--------|------|-------|---|---|
| AROM 486 C GUU A 181 194.059 181.374 9.615 1.00 17.24 A C AROM 487 O GUU A 181 183.169 180.514 9.711 1.00 17.81 A O AROM 488 N VAL A 182 184.073 182.486 10.336 1.00 16.10 A C AROM 490 CB VAL A 182 183.056 182.746 11.323 1.00 16.10 A C AROM 490 CB VAL A 182 183.056 182.746 11.323 1.00 16.10 A C AROM 490 CB VAL A 182 183.417 183.989 12.155 1.00 17.20 A C AROM 492 CG2 VAL A 182 184.675 183.709 12.948 1.00 15.06 A C AROM 492 CG2 VAL A 182 184.675 183.709 12.948 1.00 15.06 A C AROM 493 C VAL A 182 184.675 183.709 12.948 1.00 15.06 A C AROM 494 N VAL A 182 180.718 182.216 11.186 1.00 14.19 A N AROM 495 N C ALL A 182 180.718 182.216 11.186 1.00 14.19 A N AROM 495 N C ALL A 182 180.718 182.216 11.186 1.00 14.19 A N AROM 496 N C ALL A 183 180.190 185.197 8.214 1.00 16.51 A C AROM 496 N C ALL A 183 180.190 185.197 8.214 1.00 16.51 A C AROM 497 N C ALL A 183 180.190 185.197 8.214 1.00 16.51 A C AROM 497 N C ALL A 183 180.190 185.197 8.214 1.00 24.47 A C AROM 497 N C ALL A 183 180.566 187.674 7.874 1.00 24.47 A C AROM 497 N C ALL A 183 180.566 187.674 7.874 1.00 24.47 A C AROM 501 022 GUU A 183 180.566 187.674 7.874 1.00 24.47 A C AROM 501 022 GUU A 183 180.555 188.801 8.315 1.00 16.51 A AROM 503 O GEL GUU A 183 180.555 188.801 8.315 1.00 24.47 A C AROM 503 O GEL GUU A 183 180.566 187.674 7.874 1.00 24.47 A C AROM 503 O GEL GUU A 183 178.405 182.460 8.755 1.00 14.99 A C AROM 503 O GEL GUU A 183 178.405 182.460 8.755 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 178.405 182.460 8.755 1.00 14.99 A C AROM 503 O GEL GUU A 183 178.405 182.460 8.755 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.774 8.555 1.00 14.99 A C AROM 503 O GEL GUU A 183 179.581 182.99 A O O O O O O O O O O O O O O O O O O | MOTA | 484 | OE1 | GLU . | A | 181 | 1 | L88.877 | 179.898 | 10.811 | | | A | 0 |
| ARCOM 488 N VALA 182 181-075 182-146 10.323 1.00 13.24 A N RACOM 489 CA VALA 182 181-075 182-146 10.323 1.00 13.24 A N GOM 489 CA VALA 182 181-075 182-146 10.323 1.00 16.10 A C RACOM 491 CG1 VALA 182 181-075 182-146 11.323 1.00 16.10 A C RACOM 491 CG1 VALA 182 181-075 182-176 11.323 1.00 16.10 A C RACOM 491 CG1 VALA 182 181-075 182-176 11.323 1.00 11.33 A C RACOM 492 CG2 VALA 182 181-075 182-170 19.75 6 1.00 11.33 A C RACOM 493 C VALA 182 181-075 182-170 19.75 6 1.00 16.14 A C RACOM 493 C VALA 182 181-075 182-170 19.75 6 1.00 16.14 A C RACOM 494 O VALA 182 181-071 181-075 182-170 11.75 6 1.00 16.14 A C RACOM 495 CA GLUD A 183 181-071 181-082-170 11.75 6 1.00 16.14 A C RACOM 495 CA GLUD A 183 181-071 181-082-170 11.75 6 1.00 16.25 A N RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 495 CA GLUD A 183 180-190 185-187 8 .214 1.00 16.53 A C RACOM 502 CA GLUD A 183 179-581 182-764 8 .555 1.00 14.99 A C RACOM 502 CA GLUD A 183 179-581 182-764 8 .555 1.00 14.99 A C RACOM 502 CA GLUD A 183 189-391 182-764 8 .555 1.00 14.99 A C RACOM 504 N TLE A 184 180-396 182-019 7.810 1.00 1.05 3 A C RACOM 506 CB LLE A 184 180-396 182-019 7.810 1.00 1.05 3 A C RACOM 506 CB LLE A 184 180-396 182-019 7.810 1.00 1.05 A N RACOM 507 CA LLE A 184 180-396 182-019 7.810 1.00 1.05 3 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.00 1.05 A C RACOM 507 CA LLE A 184 180-396 180-180 7 .10 1.00 1.00 1.00 1.00 1.00 1.00 1. | ATOM | 485 | OE2 | GLU . | Α | 181 | 1 | 187.654 | 178.393 | 11.914 | 1.00 | 30.52 | Ą | 0 |
| AROM 488 N VALA 182 184.075 182, 486 10.336 1.00 13.24 A N AROM 499 CA VALA 182 183.055 182,746 11.323 1.00 11.324 A N GOM 499 CB VALA 182 183.055 182,746 11.323 1.00 11.324 A N GOM 491 CG1 VALA 182 182.271 184,362 13.059 1.00 17.20 A C RACOM 492 CG2 VALA 182 184.675 183.709 12.948 1.00 15.06 A C RACOM 493 C VALA 182 181.650 182,907 10.756 1.00 17.20 A C RACOM 493 C VALA 182 181.650 182,907 10.756 1.00 16.14 A C RACOM 493 C VALA 182 181.650 182,907 10.756 1.00 16.14 A C RACOM 493 C VALA 182 181.650 182,907 10.756 1.00 16.14 A C RACOM 495 N GLU A 183 181.491 183,805 9.788 1.00 15.05 A N C RACOM 495 N GLU A 183 181.491 183,805 9.788 1.00 15.03 A N C RACOM 495 N GLU A 183 180.630 186,499 8.842 1.00 16.51 A N C RACOM 497 N GLU A 183 180.630 186,499 8.842 1.00 16.51 A N C RACOM 497 N GLU A 183 180.630 186,499 8.842 1.00 12.63 A N C RACOM 500 CEL GUU A 183 180.840 186,566 187,674 7.874 1.00 24.47 A C RACOM 500 CEL GUU A 183 180.840 180.850 180.850 180.850 1.00 16.52 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 14.99 A C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 14.99 A C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.33 A C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.93 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 179,581 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 189,591 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 180,591 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 180,591 182,764 8.555 1.00 16.53 A N C RACOM 500 CEL GUU A 183 183,591 182,764 8.555 1.00 16.53 A N C | ATOM | 486 | С | GLU . | A | 181 | 1 | 184.059 | 181.374 | 9.615 | 1.00 | 17.24 | Α | С |
| AROM 489 CA VAL A 182 183.056 182.746 11.323 1.00 16.10 A C AROM 491 CS 17 VAL A 182 183.076 183.989 12.155 1.00 17.20 A C AROM 491 CS 17 VAL A 182 182.271 184.362 13.059 1.00 11.33 A C AROM 493 C VAL A 182 181.650 182.907 10.756 1.00 16.10 A C AROM 493 C VAL A 182 181.650 182.907 10.756 1.00 16.14 A C AROM 495 N GLU A 183 181.491 183.805 9.788 1.00 16.14 A C AROM 495 N GLU A 183 180.718 182.216 11.166 1.00 14.19 A C AROM 495 N GLU A 183 180.718 182.216 11.166 1.00 14.19 A C AROM 497 CB GLU A 183 180.190 185.187 8.212 1.00 16.25 A N AROM 496 CA GLU A 183 180.190 185.187 8.212 1.00 16.25 A N AROM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 499 CD GLU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 500 CEI GLU A 183 180.630 186.499 8.424 1.00 21.63 A C AROM 500 CEI GLU A 183 180.841 187.477 6.673 1.00 27.21 A C AROM 501 CEZ GLU A 183 180.841 187.477 6.673 1.00 27.21 A C AROM 503 C C GLU A 183 179.581 182.764 8.555 1.00 14.99 A C AROM 503 C C GLU A 183 179.581 182.764 8.555 1.00 14.99 A C AROM 504 N ILE A 184 180.396 182.049 8.555 1.00 16.33 A C AROM 505 CA LIE A 184 179.908 180.808 7.159 1.00 10.05 A C AROM 507 CB LIE A 184 180.904 180.302 6.094 1.00 9.02.03 A C AROM 507 CB LIE A 184 180.904 180.302 6.094 1.00 9.423 A C AROM 507 CB LIE A 184 180.904 180.302 6.094 1.00 9.423 A C AROM 507 CB LIE A 184 179.908 180.808 7.159 1.00 10.05 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.423 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.423 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.423 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.425 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.425 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.425 A C AROM 507 CB LIE A 184 179.508 180.302 6.094 1.00 9.425 A C AROM 507 CB LIE A 184 189.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 180.502 6.004 180 1 | ATOM | 487 | .0 | GLU . | A | 181 | | | | 9.711 | 1.00 | 17.81 | A | 0 |
| ATOM 490 CB VAL A 182 183.417 183.989 12.155 1.00 17.20 A C ATOM 491 CG1 VAL A 182 182.271 184.362 13.059 1.00 11.33 A C ATOM 492 CG2 VAL A 182 184.675 183.709 12.948 1.00 15.06 A C ATOM 493 C VAL A 182 184.675 183.709 12.948 1.00 15.06 A C ATOM 494 O VAL A 182 180.718 182.207 10.756 1.00 16.14 A C ATOM 495 N GLU A 183 180.198 182.207 10.756 1.00 16.14 A C ATOM 496 CA GLU A 183 180.198 182.216 11.186 1.00 14.19 A O ATOM 496 CA GLU A 183 180.196 185.187 8.212 1.00 17.30 A C ATOM 497 CB GLU A 183 180.190 185.187 8.212 1.00 17.30 A C ATOM 498 CG GLU A 183 180.190 185.187 8.212 1.00 17.30 A C ATOM 498 CG GLU A 183 180.190 185.187 8.212 1.00 17.30 A C ATOM 500 CEI GLU A 183 180.596 187.674 7.874 1.00 24.47 A C ATOM 500 CEI GLU A 183 180.818.918 8.315 1.00 21.63 A C ATOM 500 CEI GLU A 183 180.841 187.477 6.673 1.00 27.21 A O ATOM 500 CEI GLU A 183 180.841 187.477 6.673 1.00 27.41 A O ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 500 CEI GLU A 184 180.594 180.304 180. | MOTA | 488 | N | VAL . | A | 182 | : | 184.075 | 182.486 | 10.336 | 1.00 | 13.24 | Α | N |
| ATOM 491 CSI VAL A 182 182.271 184.362 13.059 1.00 11.33 A C ATOM 493 C VAL A 182 181.650 182.907 10.756 1.00 16.14 A C ATOM 494 O VAL A 182 181.650 182.907 10.756 1.00 16.14 A C ATOM 495 N GLU A 183 181.690 182.907 10.756 1.00 16.14 A C ATOM 495 N GLU A 183 181.491 183.805 9.788 1.00 16.25 A N ATOM 496 CA GLU A 183 180.190 182.216 11.186 1.00 14.19 A C ATOM 497 CB GLU A 183 180.190 184.021 9.121 1.00 17.30 A C ATOM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C ATOM 499 CD GLU A 183 180.630 186.499 8.42 1.00 21.63 A C ATOM 500 CEI GLU A 183 180.630 186.499 8.42 1.00 21.63 A C ATOM 500 CEI GLU A 183 180.630 186.499 8.42 1.00 21.63 A C ATOM 501 CEZ GLU A 183 180.590 186.499 8.42 1.00 21.63 A C ATOM 501 CEZ GLU A 183 180.590 182.747 7.874 1.00 24.477 A C ATOM 501 CEZ GLU A 183 180.590 182.746 8.555 1.00 14.49 A C ATOM 503 C C GLU A 183 179.591 182.746 8.555 1.00 14.49 A C ATOM 505 C GLU A 183 179.591 182.746 8.555 1.00 14.49 A C ATOM 505 C GLU A 183 179.591 182.746 8.555 1.00 14.49 A C ATOM 505 C GLU A 183 179.591 182.746 8.555 1.00 14.49 A C ATOM 505 C GLU A 183 179.591 182.746 8.555 1.00 14.49 A C ATOM 505 C GLU A 183 179.591 182.746 8.595 1.00 14.99 A C ATOM 505 C GLU A 183 179.591 182.746 8.595 1.00 14.99 A C ATOM 505 C GLU A 183 179.591 182.406 8.755 1.00 10.45 A C ATOM 505 C GLU A 183 179.591 182.746 8.595 1.00 14.99 A C ATOM 505 C GLU A 183 179.591 182.746 8.595 1.00 14.99 A C ATOM 505 C GLU A 183 179.591 182.746 8.595 1.00 14.99 A C ATOM 505 C GLU A 184 184 180.595 178.834 5.712 1.00 2.93 A C ATOM 507 C GZ ILE A 184 180.595 178.834 5.712 1.00 2.93 A C ATOM 506 C GLU A 184 184 180.595 178.834 5.712 1.00 2.93 A C ATOM 510 C ILE A 184 180.595 178.834 5.712 1.00 2.93 A C ATOM 510 C ILE A 184 180.595 179.390 9.026 1.00 14.41 A N ATOM 511 C GLU A 183 180.84 179.907 181.298 1.00 15.94 A C ATOM 513 C GLU A 183 180.84 179.907 181.834 5.712 1.00 12.93 A C ATOM 510 C GLU A 184 181 180.855 179.390 9.026 1.00 14.41 A N ATOM 510 C GLU A 188 180.855 179.390 9.026 1.00 14.41 A N ATOM 510 C GLU A 188 180.485 180.48 | ATOM | 489 | CA | VAL . | Α | 182 | : | 183.056 | 182.746 | 11.323 | | | A | |
| AROM 491 CG1 VAL A 182 182.271 184.362 13.059 1.00 11.33 A C AROM 493 C VAL A 182 181.650 182.907 10.756 1.00 16.104 A C AROM 494 O VAL A 182 181.650 182.907 10.756 1.00 16.14 A C AROM 495 N GUU A 183 181.690 182.216 11.186 1.00 14.19 A O AROM 495 N GUU A 183 180.718 182.216 11.186 1.00 14.19 A O AROM 495 N GUU A 183 180.718 182.216 11.186 1.00 14.19 A O AROM 496 CA GUU A 183 180.190 185.187 8.212 1.00 16.25 A N AROM 497 CB GUU A 183 180.190 185.187 8.212 1.00 16.25 A N AROM 499 CB GUU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 499 CB GUU A 183 180.190 185.187 8.214 1.00 16.51 A C AROM 499 CB GUU A 183 180.630 186.499 8.422 1.00 21.63 A C AROM 500 CEI GUU A 183 180.590 186.499 8.422 1.00 21.63 A C AROM 501 CEZ GUU A 183 180.590 182.747 76.73 1.00 27.21 A O AROM 501 CEZ GUU A 183 180.251 188.801 8.315 1.00 29.43 A O AROM 504 N ILE A 184 180.396 182.764 8.555 1.00 14.99 A C AROM 505 CA LIE A 184 180.396 182.460 8.753 1.00 16.33 A O AROM 506 CB LIE A 184 180.396 182.019 7.810 1.00 12.05 A N AROM 507 CB LIE A 184 180.596 180.302 6.091 1.00 12.05 A N AROM 507 CB LIE A 184 180.596 180.302 6.091 1.00 12.05 A N AROM 507 CB LIE A 184 180.590 180.302 6.091 1.00 12.05 A R AROM 507 CB LIE A 184 180.590 180.302 6.091 1.00 12.05 A R AROM 507 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.091 1.00 12.05 A R AROM 501 CB LIE A 184 179.508 180.302 6.000 12.00 12.74 A C AROM 501 CB LIE A 184 179.508 180.500 5.00 | | 490 | CB | VAL . | Α | 182 | : | 183.417 | 183.989 | 12.155 | 1.00 | 17.20 | A | |
| AROM 492 CS2 VAL A 182 184.675 183.709 12.948 1.00 15.06 A C AROM 494 O VAL A 182 181.650 182.907 10.756 1.00 16.14 A C AROM 495 O VAL A 182 180.718 182.216 11.186 1.00 14.19 A O AROM 495 N GLU A 183 180.718 182.216 11.186 1.00 14.19 A O AROM 495 N GLU A 183 180.718 182.216 11.186 1.00 14.19 A O AROM 496 CA GLU A 183 180.190 185.187 8.124 1.00 16.51 A C AROM 498 CG GLU A 183 180.656 185.187 8.124 1.00 16.51 A C AROM 498 CG GLU A 183 180.630 186.499 8.842 1.00 21.63 A C AROM 500 CEL GLU A 183 180.630 186.499 8.842 1.00 21.63 A C AROM 500 CEL GLU A 183 180.641 187.477 6.673 1.00 27.21 A O AROM 500 CEL GLU A 183 180.641 187.477 6.673 1.00 27.21 A O AROM 500 CEL GLU A 183 180.641 187.477 6.673 1.00 27.21 A O AROM 501 CEL GLU A 183 179.581 182.764 8.555 1.00 14.99 A C AROM 502 CC GLU A 183 179.581 182.764 8.555 1.00 14.99 A C AROM 503 C GLU A 183 179.581 182.764 8.555 1.00 14.99 A C AROM 505 CA ILE A 184 179.908 180.608 7.159 1.00 12.00 A N AROM 505 CA ILE A 184 179.908 180.608 7.159 1.00 10.45 A C AROM 506 CG ILE A 184 180.595 178.854 5.712 1.00 2.93 A C AROM 500 CG ILE A 184 180.595 178.654 5.712 1.00 2.93 A C AROM 500 CG ILE A 184 180.595 178.654 5.712 1.00 2.93 A C AROM 500 CG ILE A 184 180.595 178.654 5.712 1.00 2.93 A C AROM 500 CG ILE A 184 179.633 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C AROM 510 C ILE A 184 179.533 179.675 8.149 1.00 12 | | | CG1 | VAL | Α | 182 | : | 182.271 | 184.362 | 13.059 | 1.00 | 11.33 | Α | С |
| ATOM 493 C VAL A 182 181.650 182.907 10.756 1.00 16.14 A C ATOM 495 N GUU A 183 181.491 183.805 9.788 1.00 16.25 A N ATOM 496 CA GLU A 183 181.491 183.805 9.788 1.00 16.25 A N ATOM 496 CA GLU A 183 181.491 183.805 9.788 1.00 16.25 A N ATOM 497 CB GLU A 183 180.190 185.187 8.212 1.00 16.51 A C ATOM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C ATOM 499 CD GLU A 183 180.630 186.499 8.42 1.00 21.63 A C ATOM 500 CEI GLU A 183 180.630 186.499 8.42 1.00 21.63 A C ATOM 500 CEI GLU A 183 180.581 187.477 6.673 1.00 24.47 A C ATOM 501 CEZ GLU A 183 180.581 187.477 6.673 1.00 27.21 A C ATOM 502 C GLU A 183 180.581 187.477 6.673 1.00 29.43 A C ATOM 503 C C GLU A 183 180.255 188.801 8.315 1.00 29.43 A C ATOM 503 C C GLU A 183 179.581 182.764 8.555 1.00 16.33 A C ATOM 505 C C GLU A 183 179.591 182.764 8.555 1.00 16.33 A C ATOM 505 C C GLU A 183 179.591 182.764 8.555 1.00 16.33 A C ATOM 505 CA ILE A 184 179.908 180.808 7.159 1.00 10.45 A C ATOM 505 C C GLU A 183 179.591 182.764 8.555 1.00 10.45 A C ATOM 505 C C GLU A 183 179.591 180.209 7.80 1.00 10.45 A C ATOM 505 CA ILE A 184 179.908 180.808 7.159 1.00 10.45 A C ATOM 505 C C GLU A 183 179.591 180.209 7.80 1.00 10.45 A C ATOM 505 C C GLU A 183 179.908 180.808 7.159 1.00 10.45 A C ATOM 505 C C GLU A 183 180.904 180.302 6.94 1.00 9.02 A C ATOM 505 C C GLU A 183 180.904 180.302 6.94 1.00 9.02 A C ATOM 505 C C GLU A 184 180.904 180.302 6.94 1.00 9.02 A C ATOM 505 C C GLU A 184 180.802 181.248 4.93 1.00 4.36 A C ATOM 505 C C GLU A 185 180.804 79.907 8.135 1.00 13.03 A C C ATOM 510 C LLE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 C C LLE A 184 180.862 181.248 4.93 1.00 4.36 A C ATOM 510 C LLE A 184 180.862 181.248 4.93 1.00 15.54 A C ATOM 513 C C GLU A 185 180.585 179.977 8.135 1.00 13.03 A C C ATOM 510 C C LLE A 184 180.585 179.675 8.149 1.00 15.50 A C ATOM 510 C C LLE A 184 180.585 179.675 8.149 1.00 15.50 A C ATOM 510 C C LLE A 184 180.585 179.797 77.63 31 1.00 11.41 A N ATOM 512 C C GLU A 185 179.55 180.55 1.00 15.50 A C ATOM 510 C C GLU A 185 179.55 180.50 18 | ATOM | 492 | CG2 | VAL | A | 182 | : | 184.675 | 183.709 | 12.948 | 1.00 | 15.06 | A | С |
| ATOM 494 O VAL A 182 180.718 182.216 11.186 1.00 14.19 A O ATOM 495 N GLU A 183 180.190 183.805 9.788 1.00 16.25 A N ATOM 496 CA GLU A 183 180.190 185.187 8.214 1.00 16.51 A C ATOM 497 CB GLU A 183 180.190 185.187 8.214 1.00 16.51 A C ATOM 498 CG GLU A 183 180.190 185.187 8.214 1.00 21.63 A C ATOM 498 CD GLU A 183 180.190 185.187 8.214 1.00 21.63 A C ATOM 500 CGI GLU A 183 180.566 187.674 7.7674 1.00 21.63 A C ATOM 500 CGI GLU A 183 180.566 187.674 7.7674 1.00 21.47 A C ATOM 501 CGZ GLU A 183 180.566 188.601 8.315 1.00 21.41 A C ATOM 502 CC GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 O GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 O GLU A 183 179.581 182.764 8.555 1.00 16.33 A C ATOM 505 CA ILE A 184 180.396 182.409 7.810 1.00 10.53 A C ATOM 505 CA ILE A 184 180.396 182.409 7.810 1.00 10.53 A C ATOM 505 CG ILE A 184 180.9904 180.302 6.094 1.00 9.02 A C ATOM 506 CB ILE A 184 180.595 778.854 5.712 1.00 2.93 A C ATOM 507 CGZ ILE A 184 180.595 778.854 5.712 1.00 2.93 A C ATOM 507 CGZ ILE A 184 180.595 778.854 5.712 1.00 2.93 A C ATOM 509 CDI ILE A 184 180.595 778.854 5.712 1.00 2.93 A C ATOM 507 CGZ ILE A 184 180.595 778.854 5.712 1.00 2.93 A C ATOM 510 C ILE A 184 179.503 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.535 179.379 1.00 12.01 1.00 15.20 A ATOM 510 C ILE A 184 179.535 179.379 1.00 12.01 1.00 15.20 A ATOM 510 C ILE A 184 179.535 179.379 1.00 12.01 1.00 15.02 A C ATOM 510 C ILE A 184 179.535 179.379 1.00 12.01 1 | | 493 | С | VAL | Α | 182 | | 181.650 | 182.907 | 10.756 | 1.00 | 16.14 | A | С |
| ATOM 495 N GLU A 183 181.491 183.805 9.788 1.00 16.25 A N ATOM 497 CB GLU A 183 180.162 184.021 9.212 1.00 17.30 A C ATOM 497 CB GLU A 183 180.162 181.6167 8.214 1.00 16.51 A C ATOM 499 CG GLU A 183 180.163 186.499 8.214 1.00 16.51 A C ATOM 499 CD GLU A 183 180.630 186.499 8.214 1.00 21.63 A C ATOM 500 CSI GLU A 183 180.566 187.674 7.874 1.00 21.63 A C ATOM 501 CSZ GLU A 183 180.841 187.477 6.673 1.00 27.21 A C ATOM 501 CSZ GLU A 183 180.841 187.477 6.673 1.00 27.21 A C ATOM 502 C GLU A 183 180.841 182.764 8.555 1.00 27.21 A C ATOM 503 O GLU A 183 179.581 182.764 8.555 1.00 29.43 A C ATOM 503 O GLU A 183 179.581 182.764 8.555 1.00 29.43 A C ATOM 503 O GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 505 C A ILE A 184 180.396 182.019 7.810 1.00 12.00 A N ATOM 505 CA ILE A 184 180.396 182.019 7.810 1.00 12.00 A N ATOM 505 CA ILE A 184 180.994 180.302 6.094 1.00 9.02 A C ATOM 505 CGI ILE A 184 180.994 180.302 6.094 1.00 9.02 A C ATOM 505 CGI ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 505 CGI ILE A 184 1879.633 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 1879.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 1879.533 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 1879.533 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.633 179.375 8.149 1.00 12.74 A C ATOM 515 C G GLN A 185 180.585 179.300 9.026 1.00 14.41 A N ATOM 515 C G GLN A 185 180.585 179.300 9.026 1.00 14.41 A N ATOM 515 C G GLN A 185 180.585 179.300 9.026 1.00 14.41 A N ATOM 515 C G GLN A 185 180.585 179.300 9.026 1.00 14.41 A N ATOM 515 C G GLN A 185 181.664 176.555 171.299 9.960 1.00 14.41 A N ATOM 515 C G GLN A 185 181.664 177.935 1.00 10 15.60 A C ATOM 515 C G GLN A 185 181.664 177.935 1.00 10 15.60 A C ATOM 515 C G GLN A 185 181.664 177.935 1.00 10 15.60 A C ATOM 515 C G GLN A 185 181.664 177.935 1.00 10 15.60 A C ATOM 515 C G GLN A 185 181.676 177.937 1.00 18.62 1.00 18.64 A C ATOM 520 C G ERA 186 179.191 1.00 10.0 15.64 A C ATOM 520 C G ERA 186 179.191 1.00 10.0 15.64 A C ATOM 520 C G ERA 186 179.191 1.00 10.0 15.64 A C | | 494 | 0 | VAL | Α | 182 | | 180.718 | 182,216 | 11.186 | 1.00 | 14.19 | Α | 0 |
| ATOM 496 CA GLU A 183 180.162 184.021 9.212 1.00 17.30 A C C ATOM 498 CG GLU A 183 180.190 185.187 8.214 1.00 16.51 A C ATOM 498 CD GLU A 183 180.190 185.187 8.214 1.00 21.63 A C ATOM 500 021 GLU A 183 180.560 186.499 8.842 1.00 21.63 A C ATOM 501 022 GLU A 183 180.566 187.674 7.77 6.673 1.00 21.47 A C ATOM 501 022 GLU A 183 180.255 188.801 8.315 1.00 21.47 A C ATOM 502 CC GLU A 183 180.255 188.801 8.315 1.00 29.43 A O ATOM 502 CC GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 O GLU A 183 178.405 182.460 8.555 1.00 16.33 A C ATOM 504 N ILE A 184 180.396 182.409 7.810 1.00 12.00 A N ATOM 505 CA ILE A 184 180.396 182.409 7.810 1.00 10.45 A C ATOM 507 CC2 ILE A 184 180.994 180.808 7.159 1.00 10.45 A C ATOM 507 CC2 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.895 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.895 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.895 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 510 C ILE A 184 178.552 181.076 3.999 1.00 5.66 A C ATOM 510 C ILE A 184 179.563 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.563 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.563 179.380 9.026 1.00 14.41 A N ATOM 512 N GLU A 185 180.365 179.380 9.026 1.00 14.41 A N ATOM 515 CG GLU A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 516 CD GLU A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 516 CD GLU A 185 181.663 177.933 10.662 1.00 15.94 A C ATOM 516 CD GLU A 185 181.663 177.933 10.662 1.00 15.94 A C ATOM 516 CD GLU A 185 181.663 177.933 10.662 1.00 15.94 A C ATOM 516 CD GLU A 185 181.684 177.194 12.2072 1.00 15.56 A C ATOM 517 OEL GLU A 185 183.844 177.194 12.2072 1.00 15.56 A C ATOM 525 CG GLU A 185 183.844 177.198 12.700 1.00 15.56 A C ATOM 525 CG GLU A 185 183.844 177.198 12.700 1.00 15.56 A C ATOM 525 CG GLU A 185 183.844 177.198 12.700 1.00 15.50 A N ATOM 520 CG GLU A 185 179.390 1.00 10.00 15.46 A C ATOM 520 CG GLU A 188 179.391 179. | | 495 | N | GLU | Α | 183 | | 181.491 | 183.805 | 9.788 | 1.00 | 16.25 | A | N |
| ATOM 498 CG GLU A 183 180.630 186.499 8.842 1.00 21.63 A C ATOM 590 CD GLU A 183 180.566 187.674 7.7874 1.00 24.47 A C ATOM 500 ORI GLU A 183 180.566 187.674 7.7874 1.00 24.47 A C ATOM 501 ORI GLU A 183 180.565 188.801 8.315 1.00 27.21 A O ATOM 502 CG GLU A 183 180.255 188.801 8.315 1.00 29.43 A O ATOM 502 CG GLU A 183 178.405 182.460 8.555 1.00 14.99 A C ATOM 503 O GLU A 183 178.405 182.460 8.555 1.00 14.99 A C ATOM 503 O GLU A 183 178.405 182.460 8.555 1.00 14.99 A C ATOM 504 N ILE A 184 180.396 182.401 18.755 1.00 16.33 A O ATOM 505 CA ILE A 184 180.396 182.401 18.00 1.00 10.45 A C ATOM 506 CB ILE A 184 180.904 180.302 6.094 1.00 10.45 A C ATOM 506 CB ILE A 184 180.904 180.302 6.094 1.00 10.45 A C ATOM 506 CB ILE A 184 180.595 178.854 5.712 1.00 10.45 A C ATOM 508 CGI ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 510 C ILE A 184 178.552 181.076 3.999 1.00 5.66 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 12.74 A C ATOM 511 C ILE A 184 178.552 179.077 8.135 1.00 12.74 A C ATOM 512 N GLU A 185 180.365 179.380 9.026 1.00 14.41 A N ATOM 512 N GLU A 185 180.365 179.380 9.026 1.00 14.41 A N ATOM 514 CB GLU A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 515 CG GLU A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 516 CB GLU A 185 181.563 177.933 10.662 1.00 15.94 A C ATOM 516 CB GLU A 185 181.563 177.933 10.662 1.00 15.94 A C ATOM 516 CB GLU A 185 181.563 177.331 10.602 1.00 15.94 A C ATOM 517 CB GLU A 185 181.564 177.184 12.207 1.00 15.56 A C ATOM 517 CB GLU A 185 181.564 177.184 12.207 1.00 15.50 A N ATOM 518 CB GLU A 185 181.564 177.184 12.207 1.00 15.50 A N ATOM 518 CB GLU A 185 183.944 177.184 12.207 1.00 15.50 A N ATOM 520 CB GLU A 185 183.944 177.184 12.207 1.00 15.50 A N ATOM 520 CB GLU A 185 183.944 177.184 12.207 1.00 15.50 A N ATOM 520 CB GLU A 186 179.10 179.50 179.50 1.00 15.50 A N ATOM 520 CB GLU A 186 179.10 179.50 179.50 1.00 15.50 A N ATOM 520 CB GLU A 186 179.10 179.50 1 | | 496 | CA | GLU | Α | 183 | | 180.162 | 184.021 | 9.212 | 1.00 | 17.30 | A | |
| NOTE 100 CLU A 183 180.566 187.674 7.874 1.00 24.47 A C C C C C C C C C | ATOM | 497 | CB | GLU | Α | 183 | : | 180.190 | 185.187 | 8.214 | 1.00 | 16.51 | A | |
| ATOM 500 CE1 GLU A 183 180.841 187.477 6.673 1.00 27.21 A O ATOM 502 CE GLU A 183 180.255 188.801 8.315 1.00 29.43 A O ATOM 502 C GLU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 CO GLU A 183 178.405 182.460 8.753 1.00 16.33 A O C ATOM 504 N ILE A 184 180.396 182.400 8.753 1.00 16.33 A O ATOM 505 CA ILE A 184 180.396 182.400 7.159 1.00 10.45 A C ATOM 506 CB ILE A 184 180.396 182.019 7.810 1.00 12.00 A N ATOM 506 CB ILE A 184 180.396 182.400 7.159 1.00 10.45 A C ATOM 507 CG2 ILE A 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 507 CG2 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 182.025 181.076 3.939 1.00 5.66 A C ATOM 511 O ILE A 184 179.693 179.675 8.149 1.00 12.74 A C ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 513 CA GLN A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 513 CA GLN A 185 180.365 179.380 9.026 1.00 15.94 A C ATOM 515 CG GLN A 185 181.684 177.955 170.593 10.682 1.00 15.504 A C ATOM 516 CD GLN A 185 181.684 177.933 177.9475 10.00 15.22 A C ATOM 517 CG GLN A 185 181.684 177.933 179.977 8.135 1.00 13.03 A C ATOM 515 CG GLN A 185 181.684 177.933 179.979 9.960 1.00 15.94 A C ATOM 517 CG GLN A 185 181.684 177.933 179.979 10.682 1.00 15.94 A C ATOM 517 CG GLN A 185 181.684 177.933 12.074 1.00 16.62 A C ATOM 517 CG GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 519 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 519 C GLN A 185 183.048 177.939 10.682 1.00 15.50 A A C ATOM 519 C GLN A 185 183.048 177.979 11.424 1.00 16.62 A C ATOM 520 C GLN A 185 183.048 177.979 11.424 1.00 16.62 A C ATOM 520 C GLN A 185 177.950 177.637 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 177.950 177.637 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 177.950 177.637 17.637 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 177.950 177.637 17.855 10.00 15.76 A C ATOM 520 C GLN A 185 177.500 177.637 177.637 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 177.500 177.637 17.637 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 177.500 177.5 | ATOM | 498 | CG | GLU | A | 183 | | | | 8.842 | 1.00 | 21.63 | Α | С |
| ATOM 501 0E2 0EU A 183 180.255 186.801 8.315 1.00 29.43 A O ATOM 502 C GUU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 O GUU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 503 O GUU A 183 179.581 182.764 8.555 1.00 14.99 A C ATOM 505 CA LEA 184 180.396 182.460 8.753 1.00 16.33 A O ATOM 505 CA LEA 184 180.396 182.460 8.753 1.00 10.0 12.00 A N ATOM 505 CA LEA 184 180.396 182.2019 7.159 1.00 10.455 A C ATOM 506 CB LEA 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 507 CGZ LEA 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI LEA 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CGI LEA 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 501 C LEA 184 180.904 180.862 181.248 4.893 1.00 4.36 A C ATOM 510 C LEA 184 180.595 181.076 3.939 1.00 5.66 A C ATOM 511 C LEA 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 178.279 9.960 1.00 15.68 A C ATOM 516 CB GLN A 185 181.663 177.793 10.682 1.00 15.68 A C ATOM 516 CB GLN A 185 181.684 176.556 11.281 1.00 15.20 A C ATOM 516 CB GLN A 185 181.684 176.556 11.281 1.00 15.20 A C ATOM 517 CB GLN A 185 181.684 176.556 11.281 1.00 15.20 A C ATOM 518 NEZ GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 520 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 520 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 520 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 520 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.21 A N ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.20 A N ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.21 A N ATOM 520 C GLN A 185 179.257 178.551 10.977 1.00 14.20 A C ATOM 520 C GLN A 185 179.568 179.300 19.91 1.00 15.48 A C ATOM 520 C GLN A 185 179.568 179.300 19.91 1.00 15 | ATOM | 499 | CD | GLU | A | 183 | : | 180.566 | 187.674 | 7.874 | 1.00 | 24.47 | A | C |
| ATOM 502 C CLU A 183 179,581 182,764 8,555 1.00 14,99 A C RTOM 503 O GLU A 183 178,405 182,460 8,753 1.00 16,33 A O ATOM 504 N ILE A 184 180,396 182,019 7,810 1.00 16,200 A N ATOM 505 CA ILE A 184 179,908 180,808 7,159 1.00 10,45 A C ATOM 505 CB ILE A 184 180,996 182,019 7,810 1.00 12,00 A N ATOM 505 CB ILE A 184 180,996 180,808 7,159 1.00 9,02 A C ATOM 507 CG2 ILE A 184 180,595 178,854 5,712 1.00 2,93 A C ATOM 508 CG1 ILE A 184 180,862 181,244 4,8893 1.00 4,36 A C ATOM 509 CD1 ILE A 184 180,862 181,244 4,8893 1.00 4,36 A C ATOM 509 CD1 ILE A 184 187,633 179,675 8,149 1.00 12,74 A C ATOM 511 O ILE A 184 179,633 179,675 8,149 1.00 12,74 A C ATOM 511 O ILE A 184 179,633 179,675 8,149 1.00 12,74 A C ATOM 511 O ILE A 184 179,633 179,675 8,149 1.00 12,74 A C ATOM 513 CA GLN A 185 180,585 179,380 9,026 1.00 15,94 A C ATOM 513 CA GLN A 185 180,585 179,380 9,026 1.00 15,94 A C ATOM 515 CG GLN A 185 181,684 177,933 170,672 1.00 15,94 A C ATOM 515 CG GLN A 185 181,684 177,183 12,074 1.00 15,22 A C ATOM 516 CD GLN A 185 181,684 177,184 12,072 1.00 15,22 A C ATOM 517 CG1 GLN A 185 182,955 176,333 12,074 1.00 16,62 A C ATOM 519 C GLN A 185 183,044 177,184 12,072 1.00 19,84 A C ATOM 519 C GLN A 185 183,044 177,184 12,072 1.00 19,84 A C ATOM 519 C GLN A 185 183,044 177,194 12,072 1.00 19,84 A C ATOM 519 C GLN A 185 183,044 177,194 12,072 1.00 19,84 A C ATOM 520 C GLN A 185 183,044 175,198 12,760 1.00 15,50 A N ATOM 521 N SER A 186 179,1257 178,551 10,977 1.00 14,85 A C ATOM 522 CA SER A 186 179,134 179,178 11,244 1.00 16,62 A C ATOM 521 N SER A 186 179,134 179,198 11,424 1.00 15,24 A C ATOM 523 CB SER A 186 179,134 179,198 11,424 1.00 15,24 A C ATOM 525 C SER A 186 179,134 179,198 11,424 1.00 15,24 A C ATOM 525 C SER A 186 179,134 179,198 11,424 1.00 15,24 A C ATOM 525 C SER A 186 179,134 179,134 179,198 11,424 1.00 15,24 A C ATOM 525 C SER A 186 179,134 179,13 | ATOM | 500 | OE1 | GLU | Α | 183 | : | 180.841 | 187.477 | 6.673 | 1.00 | 27.21 | Α | 0 |
| ATOM 503 O GLU A 183 178.405 182.460 8.753 1.00 16.33 A O ATOM 504 N ILE A 184 180.396 182.019 7.810 1.00 12.00 A N ATOM 505 CA ILE A 184 180.904 180.808 7.159 1.00 10.45 A C ATOM 506 CB ILE A 184 180.904 180.808 7.159 1.00 10.45 A C ATOM 507 CG2 ILE A 184 180.904 180.808 7.159 1.00 10.45 A C ATOM 507 CG2 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CG1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.94 A C ATOM 516 CD GLN A 185 181.663 177.933 10.682 1.00 15.94 A C ATOM 516 CD GLN A 185 181.684 176.556 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 183.484 177.184 12.072 1.00 19.84 A C ATOM 518 NEZ GLN A 185 183.484 177.184 12.072 1.00 19.84 A C ATOM 519 C GLN A 185 183.484 177.184 12.072 1.00 19.84 A C ATOM 519 C GLN A 185 183.484 177.184 12.072 1.00 19.84 A C ATOM 512 N GLN A 185 183.648 175.198 12.760 1.00 15.50 A N C ATOM 520 C GLN A 185 179.577 178.537 11.339 1.00 11.63 A C ATOM 520 C GLN A 185 179.577 178.537 11.339 1.00 11.63 A C ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N C ATOM 520 C GLN A 185 179.577 178.537 179.518 10.9977 1.00 14.85 A C ATOM 520 C GLN A 185 179.577 178.537 179.518 10.9977 1.00 14.85 A C ATOM 520 C GLN A 185 179.577 178.537 179.501 1.00 14.85 A C ATOM 520 C GLN A 185 179.578 179.561 1.00 15.50 A N C ATOM 520 C GLN A 185 179.578 179.561 1.00 15.50 A N C ATOM 520 C GLN A 185 179.578 179.561 1.00 15.50 A N C ATOM 520 C GLN A 185 179.578 179.561 1.00 10.14 A N C ATOM 520 C GLN A 185 179.578 179.561 1.00 10.14 A N C ATOM 520 C GLN A 185 179.578 179.598 1.00 10.00 11.63 A C ATOM 520 C GLN A 185 179.578 179.598 1.00 10.00 11.63 A C ATOM 520 C GLN A 186 179.798 1.00 11.00 11.6 | MOTA | 501 | OE2 | GLU | A | 183 | ; | 180.255 | 188.801 | 8.315 | 1.00 | 29.43 | A | |
| ATOM 504 N ILE A 184 180.396 182.019 7.810 1.00 12.00 A N ATOM 505 CA ILE A 184 179.908 180.808 7.159 1.00 10.45 A C ATOM 506 CB ILE A 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 507 CG2 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CG1 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 509 CD1 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 509 CD1 ILE A 184 180.595 179.808 1.00 10.566 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.552 179.077 8.135 1.00 13.03 A O ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O ATOM 512 N GLN A 185 180.365 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.365 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.365 179.380 9.026 1.00 15.68 A C ATOM 515 CG GLN A 185 181.664 176.556 11.281 1.00 15.68 A C ATOM 515 CG GLN A 185 182.955 176.333 12.074 1.00 15.68 A C ATOM 516 CD GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 517 OEI GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.102 180.102 12.421 1.00 15.03 A C ATOM 524 OG SER A 186 178.102 180.102 12.421 1.00 15.24 A C ATOM 526 O SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 526 O SER A 186 178.102 180.102 12.421 1.00 15.76 A C ATOM 527 N HIS A 187 174.964 182.584 12.086 1.00 15.76 A C ATOM 527 N HIS A 187 174.964 180.942 19.00 12.25 A C ATOM 520 CB BER A 186 178.102 180.102 12.421 1.00 14.21 A N ATOM 520 CB HIS A 187 174.964 180.942 19.951 1.00 17.76 A C ATOM 530 CB HIS A 187 174.964 180.942 19.951 1.00 17.76 A C ATOM 531 CD2 HIS A 187 174.964 180.942 19.951 1.00 17.76 A C ATOM 532 CD BER A 186 177.757 177.956 12 1.00 18.89 A N ATOM 533 CB HIS A 187 174.964 180.942 19.951 | ATOM | 502 | С | GLU | Α | 183 | | 179.581 | 182.764 | 8.555 | 1.00 | 14.99 | A | С |
| ATOM 505 CA ILE A 184 179.908 180.808 7.159 1.00 10.45 A C ATOM 506 CB ILE A 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 507 CG2 ILE A 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 508 CG1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 13.03 A O ATOM 514 CB GLN A 185 181.684 176.556 11.221 1.00 15.22 A C ATOM 516 CD GLN A 185 181.684 176.556 11.221 1.00 15.22 A C ATOM 517 OEI GLN A 185 182.955 176.333 12.074 1.00 15.22 A C ATOM 517 OEI GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 183.844 177.189 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 179.557 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.137 177.637 11.339 1.00 11.63 A O ATOM 521 N SER A 186 179.134 179.799 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.799 11.424 1.00 14.21 A N ATOM 523 CB SER A 186 179.134 179.799 11.424 1.00 14.21 A N ATOM 525 C SER A 186 179.134 179.799 11.424 1.00 15.30 A C ATOM 526 O SER A 186 179.134 179.799 11.424 1.00 15.30 A C ATOM 526 O SER A 186 179.134 179.799 11.424 1.00 15.48 A C ATOM 526 O SER A 186 179.134 179.799 11.424 1.00 15.48 A C ATOM 526 O SER A 186 179.134 179.799 11.424 1.00 15.40 A C ATOM 526 C SER A 186 179.134 179.799 11.424 1.00 15.48 A C ATOM 526 C SER A 186 179.134 179.799 11.424 1.00 15.48 A C ATOM 526 C SER A 186 179.134 179.799 11.424 1.00 15.48 A C ATOM 530 CG HIS A 187 177.587 179.612 12.667 1.00 15.48 A C ATOM 530 CG HIS A 187 177.577 177.596 12 12.672 1.00 15.48 A C ATOM 530 CG HIS A 187 174.838 178.579 179.612 12.667 1.00 13.48 A C ATOM 530 CG HIS A 187 17 | MOTA | 503 | 0 | GLU | Α | 183 | | 178.405 | 182.460 | 8.753 | 1.00 | 16.33 | A | 0 |
| ATOM 506 CB ILE A 184 180.904 180.302 6.094 1.00 9.02 A C ATOM 507 CG2 ILE A 184 180.595 178.854 5.712 1.00 2.93 A C ATOM 508 CG1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 178.552 179.077 8.139 1.00 5.66 A C ATOM 510 C ILE A 184 178.552 179.077 8.139 1.00 12.74 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A D ATOM 512 N GLN A 185 180.365 179.360 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.365 179.360 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.663 177.933 10.662 1.00 15.68 A C ATOM 515 CG GLN A 185 181.664 176.556 11.281 1.00 15.50 A A TOM 515 CG GLN A 185 182.555 176.333 12.074 1.00 16.62 A C ATOM 517 OB1 GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 517 OB1 GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 518 NEZ GLN A 185 179.507 177.637 1.1339 1.00 14.85 A C ATOM 519 C GLN A 185 179.507 177.637 1.339 1.00 14.85 A C ATOM 519 C GLN A 185 179.507 177.637 1.339 1.00 14.85 A C ATOM 520 O GLN A 185 179.557 176.351 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 178.507 177.637 1.339 1.00 11.63 A O ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 524 OG SER A 186 178.102 180.102 12.421 1.00 15.24 A C ATOM 526 O SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 520 C SER A 186 178.102 180.102 12.421 1.00 16.11 A O ATOM 520 C SER A 186 178.102 180.102 12.421 1.00 15.42 A C ATOM 520 C SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 520 C SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 520 C SER A 186 178.104 180.102 12.421 1.00 14.21 A N ATOM 520 C SER A 186 178.104 180.102 180.102 12.421 1.00 15.40 A C ATOM 530 C SER A 186 178.104 180.102 180.102 12.421 1.00 15.40 A C ATOM 530 C SER A 186 177.787 179.612 12.672 1.00 15.40 A C ATOM 530 C SER A 186 177.787 179.612 12.672 1.00 15.40 A C ATOM 530 C SER A 186 177.507 177.507 179.612 1.00 16.57 A C ATOM 530 C SER A 186 177.508 179.908 10.00 12.57 A C ATOM 530 C SER A 187 174. | MOTA | 504 | N | ILE | Α | 184 | | 180.396 | 182.019 | 7.810 | 1.00 | 12.00 | Α | |
| ATOM 507 GG2 ILE A 184 180.8595 178.854 5.712 1.00 2.93 A C ATOM 508 CG1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 182.025 181.076 3.939 1.00 5.66 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 514 CB GLN A 185 180.665 178.279 9.906 1.00 15.94 A C ATOM 515 CG GLN A 185 181.663 177.933 10.662 1.00 15.94 A C ATOM 515 CG GLN A 185 181.663 177.933 10.662 1.00 15.54 A C ATOM 516 CD GLN A 185 181.663 177.933 10.662 1.00 15.52 A C ATOM 516 CD GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 517 OEL GLN A 185 183.844 177.184 12.072 1.00 19.84 A O C ATOM 518 NEZ GLN A 185 183.844 177.184 12.072 1.00 19.84 A O C ATOM 519 C GLN A 185 183.844 177.184 12.072 1.00 19.84 A O C ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.507 177.637 11.339 1.00 11.63 A O ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 525 C SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 526 O SER A 186 176.686 179.916 11.899 1.00 15.48 A C ATOM 526 O SER A 186 175.787 179.612 12.672 1.00 20.12 A O ATOM 527 N HIS A 187 176.483 180.048 10.552 1.00 15.79 A N ATOM 528 CA HIS A 187 176.483 180.048 10.552 1.00 15.79 A N ATOM 528 CA HIS A 187 176.483 180.048 10.552 1.00 15.79 A N ATOM 528 CA HIS A 187 176.483 180.048 10.552 1.00 15.79 A N ATOM 530 CG HIS A 187 176.483 180.048 10.552 1.00 15.79 A N ATOM 530 CG HIS A 187 177.554 184.349 9.911 1.00 14.22 A C ATOM 530 CG HIS A 187 177.554 182.348 9.414 1.00 14.22 A C ATOM 530 CG HIS A 187 177.554 182.348 9.414 1.00 14.22 A C ATOM 530 CG HIS A 187 177.554 182.348 9.414 1.00 14.22 A C ATOM 530 CG HIS A 187 177.554 182.348 9.414 1.00 14.22 A C ATOM 530 CG HIS A 187 1 | MOTA | 505 | CA | ILE | Α | 184 | | 179.908 | 180.808 | 7.159 | 1.00 | 10.45 | A | |
| ATOM 508 CG1 ILE A 184 180.862 181.248 4.893 1.00 4.36 A C ATOM 509 CD1 ILE A 184 182.025 181.076 3.99 1.00 5.66 A C ATOM 510 C ILE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O G ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 513 CA GLN A 185 181.684 176.552 178.279 9.960 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.568 A C ATOM 515 CG GLN A 185 181.684 176.556 11.281 1.00 15.22 A C ATOM 515 CG GLN A 185 181.684 176.556 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 183.844 177.184 12.072 1.00 18.62 A C ATOM 517 OEL GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 183.048 175.198 12.760 1.00 15.50 A N ATOM 519 C GLN A 185 179.557 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.577 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.134 179.198 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.198 11.424 1.00 14.21 A N ATOM 522 CB SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 524 OG SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 525 C SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 526 O SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 527 N HIS A 187 176.483 180.048 10.552 1.00 15.74 A C ATOM 528 CA HIS A 187 176.483 180.048 10.552 1.00 15.76 A C ATOM 529 CB HIS A 187 176.483 180.048 10.552 1.00 15.76 A C ATOM 529 CB HIS A 187 175.544 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 175.548 184.349 9.9516 1.00 15.76 A C ATOM 530 CG HIS A 187 175.548 184.349 9.9516 1.00 15.76 A C ATOM 530 CG HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CG HIS A 187 175.548 184.349 9.9516 1.00 13.11 A N ATOM 535 C HIS A 187 175.548 184.349 9.9516 1.00 13.11 A N ATOM 535 C HIS A | MOTA | 506 | CB | ILE | А | 184 | | 180.904 | 180.302 | | 1.00 | | | |
| ATOM 509 CD1 ILE A 184 182.025 181.076 3.939 1.00 5.66 A C ATOM 510 C ILE A 184 178.552 179.077 8.135 1.00 12.74 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 15.94 A C ATOM 514 CB GLN A 185 180.365 178.279 9.960 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.52 A C ATOM 516 CD GLN A 185 181.663 177.933 10.682 1.00 15.22 A C ATOM 516 CD GLN A 185 183.844 177.184 12.072 1.00 16.62 A C ATOM 517 0E1 GLN A 185 183.844 177.184 12.072 1.00 19.84 A C ATOM 519 C GLN A 185 183.844 177.184 12.072 1.00 16.62 A C ATOM 519 C GLN A 185 183.048 175.198 12.760 1.00 15.50 A N ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 523 CB SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 523 CB SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 525 C SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 525 C SER A 186 178.265 181.527 13.028 1.00 15.24 A C ATOM 525 C SER A 186 178.466 182.584 12.086 1.00 15.30 A C ATOM 525 C SER A 186 176.686 179.916 11.899 1.00 15.54 A C ATOM 525 C SER A 186 176.686 179.916 11.899 1.00 14.21 A N ATOM 528 CA HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 528 CB HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 528 CB HIS A 187 176.483 180.048 10.592 1.00 15.76 A C ATOM 530 CB HIS A 187 174.857 182.348 9.414 1.00 14.22 A C ATOM 530 CB HIS A 187 174.857 182.348 9.414 1.00 14.22 A C ATOM 530 CB HIS A 187 174.857 182.348 9.414 1.00 14.22 A C ATOM 530 CB HIS A 187 174.857 182.348 9.414 1.00 14.22 A C ATOM 530 CB HIS A 187 173.787 183.070 9.816 1.00 15.76 A C ATOM 530 CB HIS A 187 174.857 179.905 1.00 10.14 A C ATOM 530 CB HIS A 187 174.857 177.78 | MOTA | 507 | CG2 | ILE | Α | 184 | | 180.595 | 178.854 | 5.712 | 1.00 | 2.93 | A | |
| ATOM 510 C LLE A 184 179.633 179.675 8.149 1.00 12.74 A C ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.585 179.380 9.026 1.00 15.68 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.68 A C ATOM 515 CG GLN A 185 181.664 176.556 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 182.663 177.184 12.074 1.00 16.62 A C ATOM 516 CD GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 517 OEI GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.102 180.102 12.421 1.00 14.21 A N ATOM 522 CB SER A 186 178.102 180.102 12.421 1.00 15.20 A C ATOM 523 CB SER A 186 178.102 180.102 12.421 1.00 15.20 A C ATOM 523 CB SER A 186 178.626 181.527 13.028 1.00 15.24 A C ATOM 526 O SER A 186 176.686 179.916 11.898 1.00 15.48 A C ATOM 526 O SER A 186 175.787 179.612 12.672 1.00 20.12 A O ATOM 527 N HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 528 CA HIS A 187 175.153 179.908 10.018 1.00 15.76 A C ATOM 529 CB HIS A 187 175.153 179.908 10.018 1.00 15.76 A C ATOM 530 CB HIS A 187 175.153 179.908 10.018 1.00 15.76 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 10.14.55 A C ATOM 535 CB HIS A 187 175.548 184.369 9.951 1.00 10.14.55 A C ATOM 535 CB HIS A 187 175.548 184.369 9.951 1.00 10.14.55 A C ATOM 535 CB LEU A 188 175.480 176.243 9.118 1.00 14.55 A C ATOM 535 CB LEU A 188 175.480 176.243 9.118 1.00 14.55 A C ATOM 536 CB LEU A 188 175.608 176.243 9.118 1.00 17.67 A C ATOM 537 N LEU A 188 175.797 177.559 9.616 1.00 10.14 A C ATOM 536 CB LEU A 188 175.608 176.243 9.118 1.00 17.67 A C ATOM 537 N LEU A 188 175.608 176.243 9.118 1.00 17.59 A C ATOM 537 N LEU A 188 175.406 176.200 6.155 1.00 14.64 A C ATOM 537 N LEU A 188 | MOTA | 508 | CG1 | ILE | Α | 184 | | 180.862 | 181.248 | | 1.00 | | A | |
| ATOM 511 O ILE A 184 178.552 179.077 8.135 1.00 13.03 A O ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.365 178.279 9.960 1.00 15.94 A C ATOM 516 CB GLN A 185 181.663 177.933 10.682 1.00 15.94 A C ATOM 516 CB GLN A 185 181.663 177.933 10.682 1.00 15.548 A C ATOM 516 CD GLN A 185 181.663 177.6556 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 182.955 176.556 11.281 1.00 15.22 A C ATOM 517 OE1 GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 518 NE2 GLN A 185 183.048 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 179.257 178.551 10.977 1.00 14.65 A C ATOM 519 C GLN A 185 179.557 177.637 11.339 1.00 11.63 A O ATOM 520 O GLN A 185 179.557 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.106 100.102 12.421 1.00 15.30 A C ATOM 523 CB SER A 186 178.106 100.102 12.421 1.00 15.30 A C ATOM 525 C SER A 186 178.106 180.102 12.421 1.00 15.30 A C ATOM 525 C SER A 186 178.106 180.591 1.00 15.48 A C ATOM 526 O SER A 186 175.198 1.527 13.028 1.00 15.48 A C ATOM 526 C SER A 186 175.787 179.612 12.672 1.00 20.12 A O ATOM 527 N HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 528 C B HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 529 CB HIS A 187 174.857 199.602 12.672 1.00 20.12 A C ATOM 530 CG HIS A 187 174.857 182.307 9.810 1.00 15.506 A C ATOM 531 CD2 HIS A 187 174.857 182.307 9.911 1.00 14.22 A C ATOM 532 ND HIS A 187 174.857 182.307 9.951 1.00 10.14 A C ATOM 532 ND HIS A 187 174.857 182.307 9.951 1.00 15.50 A N ATOM 533 CE HIS A 187 174.857 182.348 9.414 1.00 14.55 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 10.14 A C ATOM 532 ND HIS A 187 175.548 184.369 9.951 1.00 10.14 A C ATOM 530 CG HIS A 187 174.857 182.348 9.414 1.00 14.55 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 17.67 A C ATOM 534 CE HIS A 187 175.548 184.369 9.951 1.00 17.60 A N ATOM 535 C HIS A 187 175.548 184.369 9.951 1.00 17.67 A C ATOM 530 CG HIS A 187 174.857 182.348 9.414 1.00 14.55 A C ATOM 530 CG HIS A 188 175.540 1 | MOTA | 509 | CD1 | ILE | А | 184 | | | | | | | | |
| ATOM 512 N GLN A 185 180.585 179.380 9.026 1.00 14.41 A N ATOM 513 CA GLN A 185 180.365 178.279 9.960 1.00 15.94 A C ATOM 515 CB GLN A 185 181.663 177.933 10.682 1.00 15.68 A C ATOM 516 CD GLN A 185 181.684 176.556 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 182.955 176.533 12.074 1.00 16.62 A C ATOM 517 OE1 GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.102 180.102 12.421 1.00 15.30 A C ATOM 522 CA SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 524 OS SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 525 C SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 526 O SER A 186 178.668 179.916 11.898 1.00 15.30 A C ATOM 527 N HIS A 187 176.686 179.916 11.898 1.00 15.79 A N ATOM 528 CA HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 529 CB HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 520 CB HIS A 187 174.964 180.942 8.914 1.00 14.22 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 531 CD2 HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 530 CB HIS A 187 174.964 180.942 8.914 1.00 14.55 A C ATOM 531 CD2 HIS A 187 175.594 184.329 9.516 1.00 13.11 A N ATOM 536 O G HIS A 187 175.594 184.329 9.516 1.00 14.94 A C ATOM 534 NEZ HIS A 187 175.594 184.329 9.516 1.00 14.99 A C ATOM 540 CB HIS A 187 175. | ATOM | 510 | С | | | | | | | | | | | |
| ATOM 514 CB GLN A 185 180.365 178.279 9.960 1.00 15.94 A C ATOM 514 CB GLN A 185 181.663 177.933 10.682 1.00 15.68 A C ATOM 515 CG GLN A 185 181.663 177.555 11.281 1.00 15.22 A C ATOM 516 CD GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 516 CD GLN A 185 182.955 176.333 12.074 1.00 16.62 A C ATOM 517 CB1 GLN A 185 183.844 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 183.048 177.184 12.072 1.00 19.84 A O ATOM 518 NE2 GLN A 185 183.048 175.198 12.760 1.00 15.50 A N ATOM 519 C GLN A 185 179.257 178.551 10.977 1.00 14.85 A C ATOM 520 O GLN A 185 178.507 177.637 11.339 1.00 11.63 A O ATOM 521 N SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 179.134 179.798 11.424 1.00 14.21 A N ATOM 522 CA SER A 186 178.265 181.527 13.028 1.00 15.30 A C ATOM 524 OG SER A 186 178.686 179.916 11.898 1.00 15.44 A C ATOM 525 C SER A 186 176.686 179.916 11.898 1.00 15.48 A C ATOM 525 C SER A 186 175.787 179.612 12.672 1.00 15.50 A A C ATOM 526 C SER A 186 175.787 179.612 12.672 1.00 20.12 A O ATOM 527 N HIS A 187 176.483 180.048 10.592 1.00 15.79 A N ATOM 529 CB HIS A 187 176.483 180.948 9.414 1.00 14.22 A C ATOM 520 CB HIS A 187 175.153 179.908 10.018 1.00 15.57 A C ATOM 530 CG HIS A 187 175.543 199.908 10.018 1.00 14.22 A C ATOM 530 CG HIS A 187 175.543 199.908 10.018 1.00 14.22 A C ATOM 531 CD2 HIS A 187 175.949 183.89 9.414 1.00 14.22 A C ATOM 530 CG HIS A 187 175.948 184.369 9.951 1.00 10.14 A C ATOM 530 CG HIS A 187 175.548 184.369 9.951 1.00 10.14 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 10.14.22 A C ATOM 530 CG HIS A 187 175.548 184.369 9.951 1.00 10.14.22 A C ATOM 530 CG HIS A 187 175.548 184.369 9.951 1.00 10.14.22 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 10.14.22 A C ATOM 530 CE HIS A 187 175.548 184.369 9.951 1.00 10.14 A C ATOM 531 CD2 HIS A 187 175.548 184.369 9.951 1.00 10.14 A C ATOM 534 NEE HIS A 187 175.548 184.369 9.951 1.00 12.55 A C ATOM 530 CE HIS A 187 175.548 184.369 9.951 1.00 12.55 A C ATOM 530 CE HIS A 188 175.777 177.559 9.616 1.00 12.50 A N A ATOM | MOTA | 511 | 0 | | | | | | | | | | | |
| ATOM 514 CB GLN A 185 | MOTA | | | | | | | | | | | | | |
| ATOM 515 CG GIN A 185 | MOTA | | | | | | | | | | | | | |
| ATOM 516 CD GLN A 185 | | | | | | | | | | | | | | |
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| ATOM 536 O HIS A 187 173.762 178.272 8.931 1.00 17.40 A O ATOM 537 N LEU A 188 175.777 177.595 9.616 1.00 18.89 A N ATOM 538 CA LEU A 188 175.608 176.243 9.118 1.00 16.21 A C ATOM 539 CB LEU A 188 176.972 175.721 8.652 1.00 15.40 A C ATOM 540 CG LEU A 188 177.339 175.433 7.185 1.00 14.79 A C ATOM 541 CD1 LEU A 188 176.514 176.200 6.155 1.00 14.64 A C ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 549 CD ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.190 174.086 11.398 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.193 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.598 14.091 1.00 42.31 A N | | 535 | | | | | | 174.838 | 178.515 | | 1.00 | 17.67 | A | С |
| ATOM 538 CA LEU A 188 175.608 176.243 9.118 1.00 16.21 A C ATOM 539 CB LEU A 188 176.972 175.721 8.652 1.00 15.40 A C ATOM 540 CG LEU A 188 177.339 175.433 7.185 1.00 14.79 A C ATOM 541 CD1 LEU A 188 176.514 176.200 6.155 1.00 14.64 A C ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 549 CD ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.598 14.091 1.00 43.35 A C | | 536 | 0 | HIS | Α | 187 | | | | 8.931 | 1.00 | 17.40 | A | 0 |
| ATOM 540 CG LEU A 188 176.972 175.721 8.652 1.00 15.40 A C ATOM 540 CG LEU A 188 177.339 175.433 7.185 1.00 14.79 A C ATOM 541 CD1 LEU A 188 176.514 176.200 6.155 1.00 14.64 A C ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 32.57 A C ATOM 550 NE ARG A 189 172.196 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.598 14.091 1.00 43.35 A C | ATOM | 537 | N | LEU | Α | 188 | | | | | 1.00 | 18.89 | A | Ŋ |
| ATOM 540 CG LEU A 188 177.339 175.433 7.185 1.00 14.79 A C ATOM 541 CD1 LEU A 188 176.514 176.200 6.155 1.00 14.64 A C ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | MOTA | 538 | CA | LEU | Α | 188 | | | | | 1.00 | 16.21 | A | С |
| ATOM 541 CD1 LEU A 188 176.514 176.200 6.155 1.00 14.64 A C ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | ATOM | 539 | CB | LEU | Α | 188 | | | | | | | A | |
| ATOM 542 CD2 LEU A 188 178.805 175.738 7.024 1.00 11.29 A C ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | MOTA | 540 | CG | LEU | A | 188 | | | | | 1.00 | 14.79 | A | |
| ATOM 543 C LEU A 188 175.047 175.408 10.266 1.00 17.59 A C ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | ATOM | 541 | CD1 | LEU | Α | 188 | | | | | | | A | |
| ATOM 544 O LEU A 188 175.382 175.630 11.423 1.00 19.21 A O ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | MOTA | 542 | CD2 | LEU | A | 188 | | | | | | | A | |
| ATOM 545 N ARG A 189 174.174 174.458 9.955 1.00 19.36 A N ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | ATOM | 543 | С | | | | | | | | | | | С |
| ATOM 546 CA ARG A 189 173.579 173.603 10.988 1.00 21.36 A C ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | MOTA | | 0 | | | | | | | | | | | |
| ATOM 547 CB ARG A 189 172.190 174.086 11.398 1.00 22.58 A C ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | ATOM | | | | | | | | | | | | | |
| ATOM 548 CG ARG A 189 172.131 175.420 12.110 1.00 32.57 A C ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | MOTA | | | | | | | | | | | | | |
| ATOM 549 CD ARG A 189 172.277 175.274 13.621 1.00 34.83 A C ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | | | | | | | | | | | | | | |
| ATOM 550 NE ARG A 189 172.168 176.568 14.298 1.00 40.56 A N ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | | | | | | | | 172.131 | 175.420 | | | | | |
| ATOM 551 CZ ARG A 189 172.993 177.598 14.091 1.00 43.35 A C ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | | | | | | | | | | | | | | |
| ATOM 552 NH1 ARG A 189 173.993 177.481 13.215 1.00 42.31 A N | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | |
| ATOM 553 NH2 ARG A 189 1/2.82/ 1/8./40 14.//0 1.00 42.32 A N | | | | | | | | | | | | | | |
| | MOTA | 553 | NH2 | ARG | A | 189 | | 112.827 | 1/8./40 | 14./70 | 1.00 | 42.32 | A | N |

| ATOM | 554 | С | ARG | A | 189 | 173.42 | 3 172.219 | 10.415 | 1.00 19.45 | Z | . c |
|--------------|------------|-----------|------------|---|-----|--------------------|------------------------|------------------|--------------------------|------------|-----|
| ATOM | 555 | 0 | ARG | A | 189 | 172.58 | 2 171.996 | 9.558 | 1.00 19.37 | P | |
| ATOM | 556 | N | HIS | | | 174.218 | 3 171.283 | 10.900 | 1.00 16.48 | A | N N |
| MOTA | 557 | CA | HIS | | | | 3 169.936 | 10.388 | 1.00 16.32 | A | |
| ATOM ATOM | 558 559 | CB CG | HIS HIS | | | | 5 169.868 | 9.042 | 1.00 13.06 | 7 | |
| ATOM | 560 | | HIS | | | | 3 168.517 3 167.430 | 8.403 8.584 | 1.00 8.96 1.00 9.19 | P. | |
| MOTA | 561 | | HIS | | | | 2 168.169 | 7.422 | 1.00 9.19 1.00 9.60 | ZA ZA | |
| ATOM | 562 | | HIS | | | | 7 166.929 | 7.026 | 1.00 8.25 | A | |
| ATOM | 563 | | HIS | | | | 2 166.456 | 7.717 | 1.00 10.48 | A | |
| ATOM | 564 | С | HIS | Α | 190 | 174.85 | 7 169.069 | 11.409 | 1.00 18.77 | Z A | |
| MOTA | 565 | 0 | HIS | | | | 7 169.538 | 12.110 | 1.00 19.58 | A | |
| ATOM | 566 | N | PRO | | | | 7 167.797 | 11.526 | 1.00 19.81 | A | N A |
| ATOM | 567 | CD | PRO | | | | 6 167.329 | 10.808 | 1.00 18.67 | A | |
| ATOM ATOM | 568 569 | CA CB | PRO PRO | | | | 6 166.749 | 12.430 | 1.00 18.82 | A | |
| ATOM | 570 | CG | | | 191 | | 3 165.545 3 166.147 | 12.108 11.615 | 1.00 15.98 1.00 19.49 | <i>I</i> A | _ |
| ATOM | 571 | C | | | 191 | | 2 166.383 | 12.239 | 1.00 15.63 | A A | |
| MOTA | 572 | 0 | | | 191 | | 4 165.908 | 13.167 | 1.00 16.18 | 2A | |
| ATOM | 573 | N | ASN | Α | 192 | 176.93 | 166.564 | 11.029 | 1.00 13.38 | A | |
| MOTA | 574 | CA | ASN | | | | 6 166.216 | 10.740 | 1.00 13.06 | P | |
| ATOM | 575 | CB | | | 192 | | 7 165.242 | 9.568 | 1.00 16.94 | A | |
| MOTA | 576 | CG | | | 192 | | 1 163.963 | 9.853 | 1.00 21.40 | A | |
| ATOM ATOM | 577 578 | | ASN ASN | | | | 3 163.790 5 163.062 | 9.431 | 1.00 24.81 | .A | |
| ATOM | 579 | C | | | 192 | | 9 167.407 | 10.596 10.467 | 1.00 19.25 1.00 13.65 | 2 A | |
| MOTA | 580 | ō | ASN | | | | 3 167.276 | 9.869 | 1.00 15.58 | .ZA .ZA | |
| ATOM | 581 | N | | | 193 | | 5 168.584 | 10.865 | 1.00 13.34 | | |
| ATOM | 582 | CA | | | 193 | | 169.789 | 10.734 | 1.00 12.06 | ZA. | |
| ATOM | 583 | CB | | | 193 | 178.88 | 5 170.843 | 9.814 | 1.00 11.35 | A | |
| ATOM | 584 | CG2 | | | | | 3 172.131 | 9.882 | 1.00 5.81 | A | |
| ATOM | 585 | | ILE | | | | 7 170.317 | 8.381 | 1.00 6.17 | A | |
| ATOM ATOM | 586 587 | CDI | ILE | | 193 | | 5 171.205 L 170.377 | 7.453 | 1.00 8.69 | A | |
| ATOM | 588 | Ö | | | 193 | | 3 170.540 | 12.134 12.840 | 1.00 12.85 1.00 14.90 | A A | |
| ATOM | 589 | N | LEU | | | | 170.678 | 12.530 | 1.00 13.66 | A | |
| ATOM | 590 | CA | LEU | | | | 3 171.253 | 13.839 | 1.00 14.76 | A | |
| MOTA | 591 | CB | LEU | | | 182.623 | 3 171.519 | 14.036 | 1.00 16.68 | A | |
| ATOM | 592 | CG | LEU | | | 183.117 | | 15.486 | 1.00 15.84 | A | |
| ATOM | 593 | CD1 | | | | | 170.099 | 16.000 | 1.00 14.02 | A | |
| ATOM ATOM | 594 595 | CDZ | LEU LEU | | | | 5 172.073 . 172.578 | 15.588 | 1.00 14.49 | A | |
| ATOM | 596 | Ö | LEU | | | 180.450 | | 13.964 13.070 | 1.00 16.81 1.00 18.34 | A A | |
| ATOM | 597 | N | ARG | | | 179.683 | | 15.085 | 1.00 15.08 | A | |
| MOTA | 598 | CA | ARG | Α | 195 | 178.924 | 173.924 | 15.390 | 1.00 16.45 | A | |
| ATOM | 599 | CB | ARG | | | 177.87€ | | 16.474 | 1.00 19.44 | А | |
| ATOM | 600 | CG | ARG | | | | 172.975 | 15.987 | 1.00 25.93 | A | , c |
| ATOM | 601 | CD | ARG | | | | 173.967 | 15.232 | 1.00 29.82 | A | |
| MOTA MOTA | 602 603 | NE CZ | ARG ARG | | | | 174.694 | 16.091 | 1.00 36.41 | A | |
| ATOM | 604 | | ARG | | | 175.804 | | 16.302 15.718 | 1.00 39.91 1.00 44.61 | A A | |
| ATOM | 605 | | ARG | | | 173.958 | | 17.075 | 1.00 40.14 | A | |
| ATOM | 606 | С | ARG | | | 179.787 | | 15.870 | 1.00 16.17 | A | |
| ATOM | 607 | 0 | ARG | | | 180.714 | 174.950 | 16.656 | 1.00 13.03 | A | |
| ATOM | 608 | N | LEU | | | 179.471 | | 15.341 | 1.00 17.85 | A | |
| MOTA | 609 610 | CA | LEU | | | 180.114 | | 15.749 | 1.00 16.50 | A | |
| ATOM ATOM | 611 | CB CG | LEU | | | 180.623 181.348 | | 14.572 14.959 | 1.00 13.17 | A | |
| ATOM | 612 | | LEU | | | 182.467 | | 15.910 | 1.00 15.31 1.00 13.98 | A A | |
| ATOM | 613 | | LEU | | | 181.922 | | 13.749 | 1.00 13.38 | A | |
| ATOM | 614 | C | LEU | | | 178.975 | | 16.466 | 1.00 15.90 | A | |
| ATOM | 615 | 0 | LEU | A | 196 | 178.037 | 178.767 | 15.839 | 1.00 15.06 | A | |
| ATOM | 616 | N | TYR | | | 179.062 | 178.337 | 17.791 | 1.00 18.19 | A | |
| ATOM | 617 | CA | TYR | | | 178.049 | 178.974 | 18.610 | 1.00 18.38 | A | |
| ATOM | 618 | CB | TYR | | | 178.154 | 178.464 | 20.033 | 1.00 15.79 | A | C |
| ATOM ATOM | 619 620 | CG CD1 | TYR TYR | | | 177.908 178.955 | 176.980 176.080 | 20.126 20.280 | 1.00 17.64 | A | C |
| ATOM | 621 | | TYR | | | 178.712 | 174.718 | 20.280 | 1.00 15.26 1.00 20.64 | A A | C |
| ATOM | 622 | | TYR | | | 176.607 | 176.469 | 20.054 | 1.00 20.04 | A A | c |
| ATOM | 623 | | TYR | | | 176.360 | 175.104 | 20.138 | 1.00 20.23 | A | č |
| | | | | | | | | | | | |

| MOTA | 624 | CZ | TYR | A | 197 | 1 | 77.418 | 174.242 | 20.293 | 1.00 | 20.94 | A | С |
|--------------|------------|---------|------------|---|------------|----|--------|--------------------|------------------|------|----------------|--------|--------|
| MOTA | 625 | OH | TYR | Α | 197 | 1 | 77.185 | 172.900 | 20.387 | 1.00 | 26.42 | Α | 0 |
| MOTA | 626 | С | TYR | A | 197 | 1 | 78.174 | 180.481 | 18.561 | 1.00 | 19.88 | Α | С |
| MOTA | 627 | 0 | TYR | A | 197 | | | 181.193 | 18.454 | 1.00 | 19.95 | Α | 0 |
| ATOM | 628 | N | GLY | | | | | 180.985 | 18.611 | 1.00 | 20.35 | Α | N |
| ATOM | 629 | CA | GLY | | | 1 | 79.542 | 182.425 | 18.562 | 1.00 | 20.00 | Α | С |
| MOTA | 630 | С | GLY | | | | | 182.838 | 18.642 | | 17.90 | Α | С |
| MOTA | 631 | 0 | GLY | | | | | 182.005 | 18.677 | | 19.17 | A | 0 |
| MOTA | 632 | N | | | 199 | | | 184.134 | 18.686 | | 17.72 | A | N |
| MOTA | 633 | CA | | | 199 | | | 184.593 | 18.748 | | 19.93 | Α | C |
| ATOM | 634 | CB | | | 199 | | | 184.776 | 17.325 | | 19.83 | A | C |
| MOTA | 635 | CG | | | 199 | | | 186.166 187.135 | 16.788 | | 21.41 | A | C |
| ATOM | 636 637 | CE1 | TYR TYR | | | | | 188.430 | 16.885 16.486 | | 21.65 | A | C |
| ATOM ATOM | 638 | | TYR | | | | | 186.538 | 16.266 | | 22.65 18.59 | A A | C |
| MOTA | 639 | | TYR | | | | | 187.841 | 15.862 | | 22.04 | A | č |
| ATOM | 640 | CZ | | | 199 | | | 188.787 | 15.972 | | 23.54 | Α | č |
| ATOM | 641 | OH | | | 199 | | | 190.089 | 15.557 | | 24.04 | A | ō |
| MOTA | 642 | С | TYR | Α | 199 | 1 | 82.693 | 185.910 | 19.508 | | 19.03 | A | С |
| ATOM | 643 | 0 | TYR | Α | 199 | 1. | 81.703 | 186.618 | 19.699 | 1.00 | 19.48 | A | 0 |
| MOTA | 644 | N | PHE | Α | 200 | 1 | 83.910 | 186.238 | 19.920 | 1.00 | 18.13 | A | N |
| MOTA | 645 | CA | | | 200 | | | 187.478 | 20.627 | | 17.58 | A | С |
| MOTA | 646 | CB | | | 200 | | | 187.397 | 22.091 | | 12.35 | Α | С |
| MOTA | 647 | CG | | | 200 | | | 186.344 | 22.955 | | 13.81 | A | c |
| ATOM | 648 | | PHE | | | | | 186.685 | 23.779 | | 14.44 | A | C |
| ATOM | 649 650 | | PHE | | | | | 185.033 185.731 | 22.998 24.636 | | 12.16 13.44 | A | C |
| MOTA MOTA | 651 | - | PHE | | | | | 184.075 | 23.845 | | 13.44 | A A | C |
| ATOM | 652 | CZ | | | 200 | | | 184.426 | 24.669 | | 13.42 | A | č |
| ATOM | 653 | C | | | 200 | | | 187.756 | 20.549 | | 18.86 | A | Č |
| ATOM | 654 | ō | | | 200 | | | 186.840 | 20.451 | | 24.13 | A | ō |
| ATOM | 655 | N | HIS | Α | 201 | 1 | 86.056 | 189.019 | 20.573 | | 19.06 | Α | N |
| MOTA | 656 | CA | HIS | A | 201 | 1 | 87.467 | 189.335 | 20.512 | 1.00 | 22.05 | A | С |
| ATOM | 657 | CB | | | 201 | | | 189.966 | 19.159 | 1.00 | 20.51 | A | C |
| ATOM | 658 | CG | | | 201 | | | 191.286 | 18.903 | | 18.99 | Α | С |
| ATOM | 659 | | HIS | | | | | 191.593 | 18.450 | | 19.83 | A | С |
| ATOM | 660 | | HIS | | | | | 192.478 | 18.965 | | 21.28 | A | N |
| MOTA | 661 662 | | HIS HIS | | | | | 193.459 192.948 | 18.544 | | 19.32 | A | C |
| ATOM ATOM | 663 | C | | | 201 | | | 190.279 | 18.223 21.629 | | 20.12 | A A | N C |
| ATOM | 664 | ŏ | | | 201 | | | 190.871 | 22.253 | | 23.67 | A | Ö |
| ATOM | 665 | N | | | 202 | | | 190.395 | 21.913 | | 23.03 | A | N |
| ATOM | 666 | CA | | | 202 | | | 191.331 | 22.936 | | 24.25 | A | Ċ |
| ATOM | 667 | CB | ASP | Α | 202 | 1 | 89.928 | 190.621 | 24.235 | 1.00 | 25.39 | Α | С |
| MOTA | 668 | CG | ASP | Α | 202 | | | 189.780 | 24.097 | 1.00 | 28.38 | A | С |
| ATOM | 669 | | ASP | | | | | 189.826 | 23.031 | | 34.60 | A | 0 |
| ATOM | 670 | | ASP | | | | | 189.066 | 25.067 | | 24.71 | A | 0 |
| ATOM | 671 | C | | | 202 | | | 192.148 | 22.398 | | 25.07 | A | C. |
| MOTA | 672 | O N | | | 202 203 | | | 192.235 192.733 | 21.193 | | 24.05 26.38 | A | 0 |
| ATOM ATOM | 673 674 | N CA | | | 203 | | | 193.564 | 23.287 22.856 | | 25.39 | A A | С И |
| ATOM | 675 | СВ | | | 203 | | | 194.257 | 24.082 | | 23.30 | A | C |
| ATOM | 676 | C | | | 203 | | | 192.847 | 22.039 | | 25.31 | A | Č |
| ATOM | 677 | 0 | | | 203 | | | 193.405 | 21.070 | | 24.76 | A | ō |
| ATOM | 678 | N | THR | A | 204 | 1 | 94.038 | 191.623 | 22.409 | | 24.17 | A | N |
| ATOM | 679 | CA | THR | A | 204 | 1 | 95.084 | 190.922 | 21.682 | 1.00 | 24.93 | A | C |
| ATOM | 680 | CB | | | 204 | | | 190.467 | 22.631 | | 28.17 | Α | С |
| ATOM | 681 | | THR | | | | | 189.534 | 23.582 | | 29.58 | A | 0 |
| ATOM | 682 | | THR | | | | | 191.672 | 23.364 | | 26.38 | A | C |
| MOTA | 683 | C | | | 204 | | | 189.711 | 20.869 | | 26.55 | A | C |
| ATOM ATOM | 684 685 | O N | | | 204 205 | | | 189.270 189.149 | 19.968 21.166 | | 25.70 26.89 | A A | О М |
| ATOM | 686 | CA | | | 205 | | | 188.002 | 20.382 | | 26.09 | A A | И С |
| ATOM | 687 | CB | | | 205 | | | 186.710 | 21.026 | | 29.89 | A | C |
| ATOM | 688 | CG | | | 205 | | | 186.595 | 22.508 | | 35.65 | A | Ċ |
| ATOM | 689 | CD | | | 205 | | | 186.465 | 23.174 | | 41.67 | A | č |
| ATOM | 690 | NE | | | 205 | 1 | 94.650 | 186.517 | 24.630 | | 50.08 | A | N |
| MOTA | 691 | CZ | | | 205 | | | 186.756 | 25.467 | | 53.61 | Α | С |
| ATOM | 692 | | ARG | | | | | 186.972 | 24.997 | | 54.63 | A | N |
| ATOM | 693 | NH2 | ARG | A | 205 | 1: | 95.429 | 186.782 | 26.781 | 1.00 | 57.41 | A | N |

| ATOM | 694 | С | ARG | Α | 205 | 191.56 | 187.869 | 20.036 | 1.00 23 | .76 | A | С |
|--------------|------------|---------|-----|---|------------|--------------------|--------------------|------------------|-----------------|------|--------|---------------|
| MOTA | 695 | 0 | ARG | A | 205 | | 3 188.654 | 20.478 | 1.00 26 | .35 | A | ō |
| ATOM | 696 | N | VAL | Α | 206 | 191.253 | 3 186.892 | 19.187 | 1.00 21 | . 67 | A | N |
| MOTA | 697 | CA | | | 206 | | 3 186.606 | 18.776 | 1.00 17 | | A | С |
| ATOM | 698 | CB | | | 206 | | 186.683 | 17.247 | 1.00 16 | | A | С |
| MOTA | 699 | | VAL | | | 188.235 | | 16.888 | 1.00 11 | | A | C |
| MOTA | 700 | | VAL | | | | 188.055 | 16.741 | 1.00 15 | | A | C |
| MOTA | 701 702 | 0 | | | 206 206 | 189.541 | | 19.225 | 1.00 16 | | A | C |
| MOTA MOTA | 702 | И | | | 207 | 190.380 188.308 | | 19.146 19.688 | 1.00 15 | | A | 0 |
| ATOM | 704 | CA | | | 207 | 187.866 | | 20.185 | 1.00 13 | | A A | N C |
| ATOM | 705 | CB | | | 207 | 187.555 | | 21.686 | 1.00 14 | | A | C |
| ATOM | 706 | CG | | | 207 | 188.599 | | 22.538 | 1.00 15 | | A | Ċ |
| ATOM | 707 | | TYR | | | 188.725 | | 22.565 | 1.00 15 | | A | Č |
| ATOM | 708 | CE1 | TYR | A | 207 | 189.669 | | 23.389 | 1.00 14 | | A | C |
| MOTA | 709 | CD2 | TYR | Α | 207 | 189.445 | | 23.347 | 1.00 13 | | A | С |
| ATOM | 710 | CE2 | TYR | Α | 207 | 190.393 | 184.263 | 24.174 | 1.00 15 | .70 | A | С |
| ATOM | 711 | CZ | | | 207 | 190.497 | | 24.192 | 1.00 16 | | Α | С |
| MOTA | 712 | OH | | | 207 | 191.413 | | 25.028 | 1.00 17 | | Α | 0 |
| ATOM | 713 | C | | | 207 | 186.624 | | 19.506 | 1.00 14 | | A | C |
| MOTA | 714 | 0 | | | 207 | 185.604 | | 19.390 | 1.00 14 | | A | 0 |
| MOTA MOTA | 715 716 | N CA | | | 208 208 | 186.716 185.597 | | 19.082 18.475 | 1.00 12 1.00 11 | | A | N |
| ATOM | 717 | CB | | | 208 | 186.025 | | 17.181 | 1.00 11 | | A A | C |
| ATOM | 718 | CG | | | 208 | 186.790 | | 16.101 | 1.00 12 | | A | c |
| ATOM | 719 | | LEU | | | 186.415 | | 14.759 | 1.00 13 | | A | č |
| ATOM | 720 | | LEU | | | | 182.794 | 16.118 | 1.00 17 | | A | Ċ |
| ATOM | 721 | С | LEU | Α | 208 | 185.092 | 180.162 | 19.473 | 1.00 11 | .42 | A | С |
| MOTA | 722 | 0 | LEU | A | 208 | 185.875 | 179.354 | 19.978 | 1.00 9 | . 69 | A | 0 |
| ATOM | 723 | N | | | 209 | | 180.194 | 19.753 | 1.00 11 | .10 | A | N |
| MOTA | 724 | CA | | | 209 | | 179.268 | 20.670 | 1.00 10 | | А | Ć |
| ATOM | 725 | CB | | | 209 | | 179.962 | 21.389 | 1.00 13 | | A | Ċ |
| MOTA | 726 | CG2 | | | 209 | | 178.980 | 22.422 | 1.00 10 | | A | C |
| ATOM ATOM | 727 728 | CG1 | | | 209 209 | | 181.303 182.209 | 21.979 22.621 | 1.00 14 | | A A | C |
| ATOM | 729 | CDI | | | 209 | | 3 178.124 | 19.785 | 1.00 10 | | A | C |
| ATOM | 730 | ō | | | 209 | | 178.238 | 19.040 | 1.00 13 | | A | 0 |
| MOTA | 731 | N | | | 210 | | 177.019 | 19.856 | 1.00 12 | | A | N |
| ATOM | 732 | CA | LEU | A | 210 | 183.065 | 175.867 | 19.044 | 1.00 13 | | A | С |
| MOTA | 733 | CB | LEU | Α | 210 | 184.348 | 175.383 | 18.375 | 1.00 13 | .93 | A | С |
| ATOM | 734 | CG | | | 210 | | 176.317 | 17.381 | 1.00 16 | | A | С |
| MOTA | 735 | | LEU | | | | 175.915 | 17.264 | 1.00 14 | | A | C |
| ATOM | 736 737 | CD2 | LEU | | 210 | | 176.245 | 16.022 | 1.00 12 | | A | C |
| ATOM ATOM | 738 | o | | | 210 | | 174.731 | 19.841 21.053 | 1.00 10 | | A A | C |
| ATOM | 739 | N | | | 211 | | 173.843 | 19.139 | 1.00 11 | | A | И |
| ATOM | 740 | CA | | | 211 | | 172.646 | 19.739 | 1.00 12 | | A | C |
| ATOM | 741 | CB | | | 211 | | 2 171.970 | 18.751 | 1.00 15 | | A | Č |
| MOTA | 742 | CG | | | 211 | | 170.462 | 18.927 | 1.00 16 | . 63 | A | C |
| ATOM | 743 | CD | | | 211 | | 169.783 | 17.784 | 1.00 23 | | Α | С |
| MOTA | 744 | | GLU | | | | 168.531 | 17.837 | 1.00 22 | | A | 0 |
| MOTA | 745 | | GLU | | | | 170.500 | 16.829 | 1.00 22 | | A | 0 |
| MOTA MOTA | 746 747 | C O | | | 211 211 | | 171.723 | 20.009 19.156 | 1.00 14 | | A | C |
| ATOM | 748 | N | | | 212 | | 171.133 | 21.196 | 1.00 11 | | A A | И О |
| MOTA | 749 | CA | | | 212 | | 170.247 | 21.589 | 1.00 15 | | A | C |
| ATOM | 750 | CB | | | 212 | | 170.072 | 23.108 | 1.00 16 | | A | č |
| MOTA | 751 | CG | TYR | Α | 212 | 184.387 | 168.938 | 23.679 | 1.00 18 | .16 | A | С |
| ATOM | 752 | | TYR | | | | 168.820 | 23.391 | 1.00 15 | | A | С |
| MOTA | 753 | | TYR | | | | 167.845 | 24.013 | 1.00 16 | | A | С |
| ATOM | 754 | | TYR | | | | 168.042 | 24.601 | 1.00 18 | | A | С |
| MOTA | 755 756 | | TYR | | | | 167.074 | 25.223 | 1.00 16. | | A. | C |
| ATOM | 756 757 | CZ | | | 212 | | 166.973 165.995 | 24.934 25.594 | 1.00 19 | | A | C |
| ATOM ATOM | 757 758 | OH C | | | 212 212 | | 168.889 | 20.909 | 1.00 15. | | A A | C |
| MOTA | 759 | 0 | TYR | | | | 168.259 | 20.920 | 1.00 13 | | A | 0 |
| MOTA | 760 | N | ALA | | | | 168.451 | 20.297 | 1.00 15 | | A | N |
| ATOM | 761 | CA | ALA | | | | 167.142 | 19.636 | 1.00 14. | | A | C |
| MOTA | 762 | CB | ALA | | | 185.341 | 167.270 | 18.302 | 1.00 16 | | A | C |
| MOTA | 763 | C | ALA | | | 185.417 | 166.270 | 20.615 | 1.00 16 | 61 | A | С |
| | | | | | | | | | | | | |

| ATOM | 764 | 0 | ALA | Α | 213 | : | 186.638 | 166.352 | 20.682 | 1.00 | 16.21 | A | 0 |
|--------------|------------|----------|------------|---|------------|---|--------------------|--------------------|------------------|------|----------------|--------|--------|
| ATOM | 765 | N | PRO | | | | 184.724 | | 21.380 | | 15.97 | A | N |
| ATOM | 766 | CD | PRO | | | | _ | 165.077 | 21.082 | | 15.58 | A | C |
| MOTA | 767 | CA | PRO | Α | 214 | : | 185.258 | 164.515 | 22.398 | | 15.31 | A | С |
| ATOM | 768 | CB | PRO | A | 214 | : | 184.000 | 163.837 | 22.963 | 1.00 | 14.60 | A | С |
| ATOM | 769 | CG | PRO | А | 214 | : | 182.844 | 164.624 | 22.417 | 1.00 | 17.26 | A | С |
| ATOM | 770 | С | PRO | A | 214 | | 186.319 | 163.472 | 22.000 | 1.00 | 17.90 | A | С |
| MOTA | 771 | 0 | PRO | | | | 187.172 | | 22.829 | 1.00 | 18.00 | A | 0 |
| ATOM | 772 | N | LEU | | | | 186.274 | | 20.777 | | 14.95 | Α | N |
| MOTA | 773 | CA | | | 215 | | 187.214 | | 20.362 | 1.00 | 14.66 | A | С |
| ATOM | 774 | CB | | | 215 | | 186.453 | | 19.692 | | 16.00 | A | С |
| MOTA | 775 | CG | | | 215 | | 185.316 | | 20.536 | | 22.00 | A | C |
| ATOM | 776 | CD1 | LEU | | | | 184.664 | | 19.898 | | 17.85 | A | C |
| ATOM | 777 | CD2 | | | | | 185.906 | | 21.877 | | 20.55 | A. | C |
| ATOM | 778 779 | С 0 | | | 215 215 | | 188.415 | | 19.505 | | 14.59 | A. | C |
| ATOM ATOM | 780 | N | | | 216 | | 189.093 188.691 | | 18.905 | | 14.29 | A. | 0 |
| ATOM | 781 | CA | | | 216 | | 189.836 | | 19.455 18.694 | | 16.74 14.83 | A. | C |
| MOTA | 782 | C | | | 216 | | 189.701 | | 17.184 | | 13.54 | A A | C |
| ATOM | 783 | ō | | | 216 | | 188.597 | | 16.656 | | 12.48 | A | Ö |
| ATOM | 784 | N | | | 217 | | 190.843 | | 16.497 | | 12.97 | A | И |
| ATOM | 785 | CA | | | 217 | | 190.867 | | 15.044 | | 14.08 | A | c |
| MOTA | 786 | CB | | | 217 | | 192.005 | | 14.503 | | 14.49 | A | Č |
| ATOM | 787 | OG1 | THR | | | | 193.242 | | 14.733 | | 16.68 | A | Ō |
| ATOM | 788 | CG2 | THR | Α | 217 | | 192.043 | 166.347 | 15.167 | | 10.84 | A | С |
| ATOM | 789 | С | THR | А | 217 | | 191.060 | 162.811 | 14.347 | 1.00 | 16.46 | A | C |
| MOTA | 790 | 0 | THR | Α | 217 | | 191.741 | 161.910 | 14.849 | 1.00 | 15.02 | A | 0 |
| ATOM | 791 | N | | | 218 | | 190.481 | | 13.153 | 1.00 | 16.27 | A | N |
| ATOM | 792 | CA | | | 218 | | 190.616 | | 12.340 | | 15.99 | A | С |
| MOTA | 793 | CB | | | 218 | | 189.802 | | 11.038 | | 16.57 | A | С |
| ATOM | 794 | | VAL | | | | 190.263 | | 9.999 | | 18.56 | A | С |
| ATOM | 795 | | VAL | | | | 188.339 | | 11.349 | | 11.27 | A | C |
| ATOM | 796 797 | C 0 | | | 218 | | 192.117 | | 12.051 | | 16.41 | A. | C |
| ATOM ATOM | 798 | N | | | 218 219 | | | 160.255 | 11.896 | | 15.84 | A | 0 |
| ATOM | 799 | CA | | | 219 | | | 162.509 | 12.008 11.789 | | 15.85 16.76 | A A | И |
| ATOM | 800 | CB | | | 219 | | 194.771 | | 11.908 | | 18.52 | A | C |
| ATOM | 801 | CG | | | 219 | | 196.259 | | 11.800 | | 19.33 | A | C |
| ATOM | 802 | | TYR | | | | | 163.870 | 10.570 | | 17.55 | A | Č |
| ATOM | 803 | | TYR | | | ; | 198.249 | 163.929 | 10.450 | | 23.59 | A | Č |
| ATOM | 804 | CD2 | TYR | Α | 219 | | 197.065 | 164.236 | 12.936 | 1.00 | 21.27 | A | С |
| ATOM | 805 | CE2 | TYR | | | ; | 198.454 | 164.289 | 12.834 | 1.00 | 20.92 | A | С |
| ATOM | 806 | CZ | | | 219 | | | 164.136 | 11.584 | 1.00 | 24.53 | A | С |
| ATOM | 807 | ОН | | | 219 | | | 164.188 | 11.448 | | 28.22 | A | 0 |
| MOTA | 808 | C | | | 219 | | 194.999 | | 12.826 | | 18.49 | A | С |
| ATOM | 809 | 0 | | | 219 | | | 160.888 | 12.494 | | 18.32 | A | 0 |
| ATOM | 810 | N | | | 220 | | | 161.836 | 14.086 | | 16.66 | A | N |
| ATOM | 811 812 | CA CB | | | 220 220 | | | 161.100 161.674 | 15.154 | | 19.76 | A | C |
| ATOM ATOM | 813 | CG | | | 220 | | | 160.949 | 16.514 17.669 | | 22.26 27.26 | A A | C |
| ATOM | 814 | CD | | | 220 | | | 161.124 | 17.660 | | 29.11 | A | C |
| ATOM | 815 | NE | | | 220 | | | 160.200 | 18.595 | | 32.84 | A | N |
| ATOM | 816 | CZ | | | 220 | | | 160.005 | 18.702 | | 35.53 | A | C |
| ATOM | 817 | | ARG | | | | | 160.669 | 17.931 | | 39.53 | A | N |
| ATOM | 818 | NH2 | ARG | A | 220 | | 199.449 | 159.129 | 19.594 | | 36.11 | A | N |
| MOTA | 819 | С | ARG | A | 220 | : | 194.908 | 159.608 | 15.088 | 1.00 | 19.85 | A | С |
| ATOM | 820 | 0 | | | 220 | : | 195.768 | 158.748 | 15.322 | 1.00 | 19.84 | A | 0 |
| ATOM | 821 | N | | | 221 | : | 193.661 | 159.309 | 14.746 | 1.00 | 19.44 | A | N |
| ATOM | 822 | CA | | | 221 | | | 157.935 | 14.628 | | 21.14 | A | C |
| ATOM | 823 | CB | | | 221 | | | 157.930 | 14.386 | | 22.94 | A | С |
| ATOM | 824 | CG | | | 221 | | | 156.594 | 14.519 | | 27.24 | A | С |
| ATOM | 825 | CD | GLU | | | | | 155.998 | 15.918 | | 30.92 | A | C |
| ATOM | 826 927 | | GLU | | | | | 154.798 | 16.073 | | 35.57 | A | 0 |
| ATOM ATOM | 827 828 | C C | GLU GLU | | | | | 156.716 157.268 | 16.857 | | 31.40 | A | 0 |
| ATOM | 828 829 | 0 | GLU | | | | | 157.268 | 13.465 13.493 | | 22.03 21.79 | A n | C |
| ATOM | 830 | Ŋ | LEU | | | | | 158.060 | 12.442 | | 20.91 | A A | O M |
| ATOM | 831 | CA | LEU | | | | | 157.533 | 11.287 | | 18.01 | A | N C |
| ATOM | 832 | СВ | LEU | | | | | 158.485 | 10.079 | | 17.83 | A | C |
| ATOM | 833 | CG | LEU | | | | | 157.923 | 8.676 | | 21.87 | A | Č |
| | | | | | | | | _ | | | | | - |

| MOTA | 834 | CD1 | LEU | A | 222 | 194.366 | | 8.358 | 1.00 | 17.44 | A | . С |
|--------------|------------|----------|------------|---|------------|--------------------|--------------------|------------------|------|----------------|------------|------------|
| MOTA | 835 | CD2 | LEU | | | 194.892 | 159.007 | 7.634 | | 19.79 | A | |
| ATOM | 836 | С | LEU | | | 196.439 | 157.261 | 11.639 | | 16.91 | A | |
| ATOM | 837 | 0 | LEU | | | 197.012 | 156.317 | 11.119 | | 16.89 16.66 | A | |
| MOTA | 838 | N | GLN | | | 197.062 198.446 | 158.066 157.769 | 12.503 12.900 | | 17.24 | A A | |
| ATOM | 839 840 | CA CB | GLN GLN | | | 199.022 | 158.808 | 13.850 | | 19.18 | A | |
| ATOM ATOM | 841 | CG | GLN | | | 199.022 | 160.205 | 13.317 | | 28.34 | Ā | |
| ATOM | 842 | CD | GLN | | | 199.954 | 161.058 | 14.355 | | 31.88 | A | |
| ATOM | 843 | | GLN | | | 199.437 | 161.241 | 15.474 | | 31.86 | A | |
| ATOM | 844 | | GLN | | | 201.149 | 161.584 | 14.005 | | 34.43 | A | |
| ATOM | 845 | С | GLN | Α | 223 | 198.456 | 156.448 | 13.688 | 1.00 | 21.01 | ZA. | C |
| MOTA | 846 | 0 | GLN | A | 223 | 199.360 | 155.630 | 13.523 | | 18.77 | A | |
| ATOM | 847 | N | LYS | | | 197.464 | 156.277 | 14.570 | | 21.30 | Z | |
| ATOM | 848 | CA | LYS | | | 197.357 | 155.099 | 15.419 | | 21.07 | A | |
| MOTA | 849 | CB | LYS | | | 196.258 | 155.300 | 16.492 | | 24.80 | <i>Z</i> A | |
| ATOM | 850 | CG | LYS | | | 196.479 | 156.522 | 17.399 | | 26.43 | .P. | |
| ATOM | 851 | CE | LYS LYS | | | 195.427 195.834 | 156.642 157.727 | 18.505 19.507 | | 31.44 | 24 | |
| MOTA MOTA | 852 853 | NZ | LYS | | | 194.917 | 157.868 | 20.668 | | 33.32 | P | |
| ATOM | 854 | C | LYS | | | 197.088 | 153.812 | 14.647 | | 20.29 | P | |
| ATOM | 855 | ō | LYS | | | 197.799 | 152.829 | 14.821 | 1.00 | 19.90 | P | 0 |
| MOTA | 856 | N | LEU | Α | 225 | 196.059 | 153.800 | 13.806 | 1.00 | 20.45 | P | N N |
| MOTA | 857 | CA | LEU | Α | 225 | 195.753 | 152.603 | 13.039 | | 18.46 | F | |
| ATOM | 858 | CB | LEU | | | 194.272 | 152.588 | 12.615 | | 20.03 | F | |
| ATOM | 859 | CG | LEU | | | 193.224 | 152.691 | 13.740 | | 24.89 | P | |
| MOTA | 860 | | LEU | | | 191.784 | 152.656 | 13.213 | | 20.57 | F | |
| ATOM | 861 | | LEU LEU | | | 193.462 196.631 | 151.543 152.464 | 14.674 11.780 | | 26.58 19.83 | I I | |
| ATOM ATOM | 862 863 | C O | LEU | | | 196.694 | 151.381 | 11.186 | | 20.09 | Į | |
| ATOM | 864 | N | SER | | | 197.296 | | 11.375 | | 18.33 | Į | |
| ATOM | 865 | CA | SER | | | 198.137 | 153.578 | 10.158 | | 21.51 | F | |
| ATOM | 866 | СВ | SER | | | 199.160 | 152.426 | 10.124 | 1.00 | 21.48 | P | . C |
| ATOM | 867 | OG | SER | Α | 226 | 200.116 | 152.533 | 11.177 | 1.00 | 27.63 | I | |
| MOTA | 868 | С | SER | | | 197.295 | 153.542 | 8.871 | | 20.48 | Į | |
| ATOM | 869 | 0 | SER | | | 197.566 | | 7.927 | | 19.41 | F | |
| ATOM | 870 | N | LYS | | | 196.290 | 152.664 | 8.838 | | 20.02 | Į | |
| ATOM | 871 872 | CA CB | LYS | | | 195.358 195.668 | 152.524 151.280 | 7.697 6.876 | | 19.86 24.72 | 7 | |
| ATOM ATOM | 873 | CG | LYS | | | 196.854 | 151.260 | 5.990 | | 29.64 | Į | |
| ATOM | 874 | CD | LYS | | | 197.148 | | 5.419 | | 35.21 | 7 | |
| MOTA | 875 | CE | LYS | | | 198.330 | 150.088 | 4.465 | 1.00 | 41.32 | 1 | |
| ATOM | 876 | NZ | LYS | Α | 227 | 198.843 | 148.758 | 4.016 | 1.00 | 43.82 | I | |
| ATOM | 877 | C | LYS | | | 193.970 | 152.303 | 8.274 | | 16.62 | Į | |
| ATOM | 878 | 0 | LYS | | | 193.852 | 151.881 | 9.411 | | 18.80 | Į | |
| MOTA | 879 | N | PHE | | | 192.930 | | 7.499 | | 14.54 15.70 | Į. | |
| ATOM | 880 881 | CA CB | PHE PHE | | | 190.665 | 152.342 153.590 | 7.932 7.729 | | 12.09 | I | |
| ATOM ATOM | 882 | CG | | | 228 | 190.958 | | 8.679 | | 13.97 | 7 | |
| ATOM | 883 | | PHE | | | | 156.005 | 8.400 | | 14.03 | 7 | |
| ATOM | 884 | | PHE | | | | 154.439 | 9.860 | 1.00 | 13.49 | Z | A C |
| ATOM | 885 | CE1 | PHE | Α | 228 | | 157.046 | 9.299 | | 12.37 | Į | |
| MOTA | 886 | | PHE | | | | 155.466 | 10.767 | | 14.79 | 1 | |
| ATOM | 887 | CZ | | | 228 | | 156.772 | 10.487 | | 11.50 | | <i>y</i> C |
| ATOM | 888 | C | | | 228 | | 151.227 151.212 | 7.016 5.833 | | 15.70 16.89 | 7 | |
| ATOM ATOM | 889 890 | N O | | | 228 229 | | 150.290 | 7.536 | | 16.61 | | A N |
| ATOM | 891 | CA | ASP | | | | 149.221 | 6.666 | | 18.23 | | . C |
| ATOM | 892 | СВ | | | 229 | | 148.005 | 7.478 | | 17.42 | | . C |
| ATOM | 893 | CG | ASP | A | 229 | | 148.325 | 8.369 | 1.00 | 20.41 | Į | A C |
| ATOM | 894 | | ASP | | | | 149.024 | 7.930 | | 28.20 | | A O |
| ATOM | 895 | | ASP | | | | 147.859 | 9.511 | | 26.24 | | 4 0 |
| ATOM | 896 | C | | | 229 | | 149.817 | 5.810 | | 16.57 | Į | |
| ATOM | 897 | 0 | | | 229 | | 151.006 | 5.939 | | 17.37 | 7 | |
| ATOM | 898 899 | N CA | GLU | | 230 | | 149.020 149.560 | 4.952 4.084 | | 15.33 17.43 | I I | |
| ATOM ATOM | 900 | CB | | | 230 | | 149.560 | 3.002 | | 16.24 | F. | |
| ATOM | 901 | CG | | | 230 | | 148.066 | 2.153 | | 23.01 | Į | |
| ATOM | 902 | CD | | | 230 | | 147.497 | 0.794 | | 27.22 | Į | |
| ATOM | 903 | OE1 | GLU | | | 186.584 | 146.478 | 0.753 | | 28.49 | Z | |
| | | | | | | | | | | | | |

| MOTA | 904 | OE2 | GLU | A | 230 | 187.711 | 148.085 | -0.244 | 1.00 29.45 | A | 0 |
|--------------|------------|------------|------------|----|------------|---------|--------------------|-----------------|--------------------------|--------|--------|
| ATOM | 905 | С | GLU | | | 185.680 | 150.062 | 4.783 | 1.00 16.70 | A | С |
| ATOM | 906 | 0 | GLU | | | | 151.099 | 4.419 | 1.00 13.33 | A | 0 |
| ATOM | 907 | N | GLN | | | | 149.326 | 5.782 | 1.00 16.53 | A | И |
| MOTA | 908 | CA | GLN | | | | 149.711 | 6.512 | 1.00 17.02 | A | С |
| MOTA | 909 | CB | GLN | | | | 148.656 | 7.596 | 1.00 15.32 | A | |
| ATOM | 910 | CG | GLN GLN | | | | 148.737 149.841 | 8.289 9.359 | 1.00 17.56 1.00 22.59 | A A | C C |
| ATOM | 911 912 | CD OF 1 | GLN | | | | 150.112 | 10.075 | 1.00 22.39 | A | |
| ATOM ATOM | 913 | | GLN | | | | 150.112 | 9.494 | 1.00 19.70 | A | |
| ATOM | 914 | C | GLN | | | | 151.124 | 7.120 | 1.00 17.00 | A | |
| ATOM | 915 | ō | GLN | | | | 152.024 | 6.890 | 1.00 18.40 | A | |
| ATOM | 916 | N | ARG | | | | 151.308 | 7.873 | 1.00 17.36 | A | |
| ATOM | 917 | CA | ARG | A, | 232 | 185.607 | 152.593 | 8.509 | 1.00 17.63 | A | С |
| ATOM | 918 | CB | ARG | Α | 232 | 186.905 | 152.465 | 9.307 | 1.00 19.87 | A | |
| MOTA | 919 | CG | ARG | Α | 232 | 187.205 | 153.647 | 10.172 | 1.00 20.99 | A | |
| ATOM | 920 | CD | | | 232 | | 153.359 | 11.597 | 1.00 28.38 | A | |
| ATOM | 921 | NE | | | 232 | | 154.189 | 12.487 | 1.00 32.23 | A | |
| ATOM | 922 | CZ | | | 232 | | 153.745 | 13.545 | 1.00 31.41 | A | |
| MOTA | 923 | | ARG | | | | 152.459 | 13.873 | 1.00 29.13 | A | |
| ATOM | 924 | | ARG | | 232 | | 154.604 153.747 | 14.257 7.507 | 1.00 35.98 | A | |
| MOTA | 925 926 | 0 | | | 232 | | 153.747 | 7.761 | 1.00 14.94 1.00 12.98 | A A | |
| ATOM ATOM | 927 | N | | | 233 | | 153.457 | 6.384 | 1.00 12.30 | A | |
| ATOM | 928 | CA | | | 233 | | 154.446 | 5.361 | 1.00 13.60 | A. | |
| ATOM | 929 | СВ | | | 233 | | 153.902 | 4.340 | 1.00 14.55 | A | |
| ATOM | 930 | | THR | | | | 153.623 | 5.048 | 1.00 14.87 | A | |
| ATOM | 931 | CG2 | THR | Α | 233 | 188.016 | 154.908 | 3.231 | 1.00 13.20 | A | С |
| ATOM | 932 | С | THR | Α | 233 | 185.339 | 154.863 | 4.686 | 1.00 13.47 | A | С |
| MOTA | 933 | 0 | | | 233 | | 156.056 | 4.508 | 1.00 12.81 | A | |
| MOTA | 934 | N | | | 234 | | 153.901 | 4.353 | 1.00 11.54 | A | |
| ATOM | 935 | CA | | | 234 | | 154.225 | 3.713 | 1.00 12.90 | A | |
| ATOM | 936 | CB | | | 234 | | 152.967 | 3.184 | 1.00 6.31 | A | |
| ATOM | 937 938 | С 0 | | | 234 234 | | 154.953 155.843 | 4.675 4.272 | 1.00 15.13 1.00 18.25 | A A | |
| ATOM ATOM | 939 | N | | | 235 | | 154.579 | 5.945 | 1.00 13.08 | A | |
| ATOM | 940 | CA | | | 235 | | 155.221 | 6.909 | 1.00 11.34 | A | |
| ATOM | 941 | СВ | | | 235 | | 154.543 | 8.289 | 1.00 13.04 | A | |
| ATOM | 942 | | THR | | | | 153.167 | 8.177 | 1.00 13.03 | A | |
| ATOM | 943 | CG2 | THR | A | 235 | | 155.235 | 9.304 | 1.00 9.30 | A | |
| ATOM | 944 | С | | | 235 | | 156.701 | 6.976 | 1.00 12.76 | A | |
| MOTA | 945 | 0 | | | 235 | | 157.553 | 6.894 | 1.00 14.21 | A | |
| ATOM | 946 | N | | | 236 | | 157.003 | 7.115 | 1.00 12.83 | A | |
| ATOM | 947 | CA | | | 236 236 | | 158.392 158.451 | 7.157 7.371 | 1.00 14.72 1.00 16.17 | A | |
| ATOM ATOM | 948 949 | CB CG | | | 236 | | 158.175 | 8.772 | 1.00 16.17 | A A | |
| ATOM | 950 | | TYR | | | | 158.491 | 9.876 | 1.00 16.03 | A | |
| ATOM | 951 | | TYR | | | | 158.261 | 11.162 | 1.00 16.90 | A | |
| ATOM | 952 | | TYR | | | | 157.626 | 8.993 | 1.00 13.79 | A | |
| ATOM | 953 | CE2 | TYR | Α | 236 | 187.290 | 157.397 | 10.266 | 1.00 15.98 | A | |
| ATOM | 954 | cz | TYR | Α | 236 | 186.490 | 157.709 | 11.347 | 1.00 19.04 | A | С |
| ATOM | 955 | OH | | | 236 | | 157.420 | 12.609 | 1.00 22.33 | A | |
| MOTA | 956 | С | | | 236 | | 159.154 | 5.862 | 1.00 16.50 | A | |
| ATOM | 957 | 0 | | | 236 | | 160.311 | 5.898 | 1.00 15.39 | A | |
| ATOM | 958 | N | | | 237 | | 158.517 | 4.718 | 1.00 14.99 | A | |
| ATOM ATOM | 959 960 | CA CB | | | 237 237 | | 159.176 158.295 | 3.456 2.242 | 1.00 15.34 1.00 15.72 | A A | |
| ATOM | 961 | | ILE | | | | 159.027 | 0.960 | 1.00 13.72 | A | |
| ATOM | 962 | | ILE | | | | 157.993 | 2.241 | 1.00 13.11 | A | |
| ATOM | 963 | | ILE | | | | 159.254 | 2.278 | 1.00 13.67 | A | |
| ATOM | 964 | C | | | 237 | | 159.542 | 3.379 | 1.00 17.56 | A | |
| MOTA | 965 | 0 | | | 237 | | 160.638 | 2.953 | 1.00 18.55 | A | |
| ATOM | 966 | N | THR | A | 238 | | 158.626 | 3.804 | 1.00 17.36 | A | |
| MOTA | 967 | CA | | | 238 | | 158.853 | 3.816 | 1.00 14.99 | Α | |
| ATOM | 968 | CB | | | 238 | | 157.600 | 4.330 | 1.00 13.08 | A | |
| ATOM | 969 | | THR | | | | 156.502 | 3.464 | 1.00 16.26 | A | |
| MOTA | 970 | | THR | | | | 157.817 | 4.354 4.696 | 1.00 13.58 | A | |
| MOTA | 971 972 | С 0 | | | 238 | | 160.829 | 4.696 | 1.00 14.23 1.00 14.27 | A A | |
| ATOM ATOM | 972 | Ŋ | | | 238 239 | | 160.829 | 5.888 | 1.00 14.27 | A A | |
| ATOM | 213 | 7.4 | ∪ىرى | М | 237 | 4/2.043 | | 5.555 | T.00 TI.03 | ~ | FA |

| | | | | | | | 50/75 | | | | | | |
|--------------|--------------|-----------|------------|---|------------|---------|------------------------|------------------|------|----------------|---|--------|--------|
| ATOM | 974 | CA | GLU | A | 239 | 179.285 | 161.242 | 6.781 | 1.00 | 13.23 | | A | С |
| MOTA | 975 | CB | GLU | | | | 161.025 | 8.170 | | 14.00 | | A | С |
| MOTA | 976 | CG | GLU | | | | 159.721 | 8.804 | | 18.38 | | A | C |
| MOTA | 977 978 | CD | GLU | | | | 159.365 159.259 | 10.124 10.187 | | 24.00 | | A A | CO |
| ATOM ATOM | 979 | | GLU | | | | 159.259 | 11.114 | | 32.52 | | A. | o |
| ATOM | 980 | C | GLU | | | | 162.548 | 6.149 | | 13.27 | | A | C |
| MOTA | 981 | ō | GLU | | | | 163.525 | 6.073 | | 12.45 | | A | ō |
| ATOM | 982 | N | LEU | | | 181.005 | 162.538 | 5.668 | 1.00 | 11.05 | | A | N |
| ATOM | 983 | CA | LEU | | | | 163.707 | 5.049 | | 13.29 | | A. | С |
| MOTA | 984 | CB | LEU | | | | 163.465 | 4.738 | | 15.79 | | A | C |
| MOTA | 985 986 | CG CD1 | LEU | | | | 164.638 | 4.235 5.279 | | 16.19 19.17 | | A A | C |
| ATOM ATOM | 987 | | LEU | | | | 164.108 | 3.884 | | 19.04 | | A A | c |
| ATOM | 988 | C | LEU | | | | 164.081 | 3.773 | | 13.39 | | A | C |
| MOTA | 989 | 0 | LEU | A | 240 | 180.513 | 165.256 | 3.548 | 1.00 | 14.19 | , | A | 0 |
| MOTA | 990 | N | ALA | | | | 163.091 | 2.955 | | 11.67 | | A | N |
| ATOM | 991 | CA | | | 241 | | 163.372 | 1.711 | | 12.50 | | A | C |
| MOTA | 992 993 | CB C | | | 241 241 | | 162.108 | 0.873 1.979 | 1.00 | 9.22 | | A n | C C |
| ATOM ATOM | 993 | 0 | | | 241 | | 164.004 | 1.222 | | 14.45 | | A A | 0 |
| ATOM | 995 | N | | | 242 | | 163.562 | 3.053 | | 14.82 | | A | N |
| MOTA | 996 | CA | | | 242 | | 164.109 | 3.447 | 1.00 | 16.37 | | A | С |
| MOTA | 997 | CB | | | 242 | | 163.329 | 4.619 | | 20.05 | | A | С |
| ATOM | 998 | CG | | | 242 | | 162.005 | 4.210 | | 22.16 | | A. | C |
| MOTA MOTA | 999 1000 | | ASN ASN | | | | 161.133 161.850 | 5.055 2.922 | | 23.63 | | A A | O N |
| ATOM | 1001 | C | | | 242 | | 165.540 | 3.918 | | 16.87 | | A | C |
| ATOM | 1002 | 0 | | | 242 | | 166.429 | 3.636 | | 13.50 | | A | 0 |
| MOTA | 1003 | N | | | 243 | | 165.747 | 4.656 | | 13.07 | | A | N |
| ATOM | 1004 | CA | | | 243 | | 167.065 | 5.190 | | 13.28 | | A | C |
| ATOM | 1005 | CB C | | | 243 | | 166.982 | 6.137 4.072 | | 13.95 14.76 | | A A | C |
| MOTA MOTA | 1006 1007 | 0 | | | 243 243 | | 168.063 | 4.072 | | 11.54 | | A A | 0 |
| ATOM | 1008 | N | | | 244 | | 167.651 | 3.113 | | 15.34 | | A | N |
| ATOM | 1009 | CA | LEU | Α | 244 | 179.487 | 168.477 | 1.955 | 1.00 | 14.00 | | A | С |
| ATOM | 1010 | CB | | | 244 | | 167.766 | 1.134 | | 12.82 | | A | С |
| ATOM | 1011 | CG | | | 244 | | 167.607 | 1.791 | | 13.66 | | A | C |
| ATOM ATOM | 1012 1013 | | LEU LEU | | | | 2 166.784 3 168.990 | 0.883 2.068 | | 10.60 | | A A | C |
| ATOM | 1014 | C | | | 244 | | 168.764 | 1.078 | | 13.84 | | A | c |
| MOTA | 1015 | 0 | | | 244 | | 169.862 | 0.545 | 1.00 | 9.94 | | A | 0 |
| ATOM | 1016 | N | | | 245 | | 167.776 | 0.949 | | 11.65 | | A | N |
| MOTA | 1017 | CA | | | 245 | | 2 167.951 | 0.149 | | 12.45 | | A - | C |
| MOTA MOTA | 1018 1019 | CB OG | | | 245 245 | | 3 166.623 5 166.724 | 0.101 | | 11.63 18.58 | | A A | 0 |
| ATOM | 1020 | C | | | 245 | | 169.090 | 0.716 | | 12.58 | | A | c |
| ATOM | 1021 | Ō | | | 245 | | 169.925 | -0.028 | | 13.38 | | A | ō |
| MOTA | 1022 | N | TYR | Α | 246 | | 169.126 | 2.038 | 1.00 | 10.82 | | A | N |
| ATOM | 1023 | CA | | | 246 | | 3 170.146 | 2.719 | | 12.87 | | A | C |
| ATOM ATOM | 1024 1025 | CB CG | | | 246 246 | | 169.838 | 4.232 5.076 | | 10.92 13.12 | | A A | C |
| ATOM | 1025 | | TYR | | | | 171.318 | 5.169 | | 11.79 | | A | C |
| ATOM | 1027 | | TYR | | | | 172.526 | 5.886 | | 15.75 | | A | Ċ |
| ATOM | 1028 | | TYR | | | | 171.782 | 5.727 | | 14.34 | | A | С |
| MOTA | 1029 | | TYR | | | | 172.925 | 6.452 | | 17.65 | | A | C |
| ATOM | 1030 1031 | CZ | | | 246 246 | | 3 173.288 5 174.411 | 6.526 7.231 | | 18.09 | | A N | C |
| ATOM ATOM | 1031 | OH C | | | 246 | | 171.506 | 2.474 | | 20.69 | | A A | 0 |
| MOTA | 1033 | ō | | | 246 | | 172.522 | 2.263 | | 16.54 | | A | ŏ |
| ATOM | 1034 | N | | | 247 | 176.398 | 171.506 | 2.526 | | 12.79 | | A | Ŋ |
| ATOM | 1035 | CA | | | 247 | | 172.695 | 2.312 | | 15.14 | | A. | C |
| ATOM | 1036 | CB | | | 247 | | 172.339 | 2.453 | | 18.30 | | A. | С |
| ATOM ATOM | 1037 1038 | SG C | | | 247 247 | | 172.397 | 4.097 0.930 | | 20.02 | | A A | s C |
| ATOM | 1038 | 0 | | | 247 | | 174.517 | 0.765 | | 13.32 | | A. | 0 |
| ATOM | 1040 | N | | | 248 | | 172.424 | -0.063 | | 12.96 | | A | N |
| ATOM | 1041 | CA | | | 248 | 176.867 | 172.853 | -1.435 | 1.00 | 14.92 | | A | С |
| ATOM | 1042 | CB | | | 248 | | 171.711 | -2.361 | | 14.58 | | A | C |
| ATOM | 1043 | CG | HIS | A | 248 | 178.698 | 171.388 | -2.305 | 1.00 | 15.75 | i | A. | С |

| MOTA | 1044 | CD2 | HIS | Α | 248 | 179.65 | 1 | 171.777 | -1.427 | 1.00 | 14.69 | Α | С |
|-------|------|-----|-----|---|-----|--------|---|--------------------|-----------------|------|-------|----|---|
| ATOM | 1045 | ND1 | HIS | A | 248 | 179.33 | Ĺ | 170.596 | -3.236 | 1.00 | 18.18 | A | N |
| ATOM | 1046 | CE1 | HIS | Α | 248 | 180.61 | 4 | 170.512 | -2.934 | 1.00 | 15.22 | A | С |
| ATOM | 1047 | NE2 | HIS | Α | 248 | 180.83 | 2 | 171.220 | -1.840 | 1.00 | 14.77 | A | N |
| MOTA | 1048 | С | HIS | Α | 248 | 175.47 | 4 | 173.338 | -1.717 | 1.00 | 16.00 | Α | С |
| ATOM | 1049 | ō | HIS | | | | | 174.228 | -2.538 | 1.00 | 16.44 | A | 0 |
| ATOM | 1050 | N | SER | | | | | 172.744 | -1.028 | | 14.49 | A | Ŋ |
| ATOM | 1051 | CA | SER | | | | | 173.148 | -1.197 | | 15.32 | A | C |
| MOTA | 1052 | CB | SER | | | | | 172.233 | -0.392 | | 11.40 | A | Č |
| ATOM | 1052 | OG | SER | | | | | 172.527 | 0.985 | | 16.48 | A | ő |
| | | | - | | | | | 174.597 | -0.696 | | 16.09 | A | C |
| MOTA | 1054 | C | SER | | | | | | | | 18.04 | A | 0 |
| ATOM | 1055 | 0 | SER | | | | | 175.350 | -1.034 0.118 | | | | N |
| MOTA | 1056 | N | LYS | | | | | 174.988 176.363 | | | 15.99 | A | C |
| ATOM | 1057 | CA | LYS | | | | _ | | 0.599 | | 15.13 | A | |
| ATOM | 1058 | CB | LYS | | | | | 176.441 | 2.107 | | 13.57 | A | C |
| MOTA | 1059 | CG | LYS | | | | | 175.850 | 3.040 | | 15.19 | A | C |
| ATOM | 1060 | CD | LYS | | | | | 176.203 | 2.629 | | 19.05 | A. | C |
| ATOM | 1061 | CE | LYS | | | | | 175.150 | 3.131 | | 24.43 | A | С |
| MOTA | 1062 | ΝZ | LYS | | | | | 175.372 | 2.776 | | 28.76 | A | N |
| MOTA | 1063 | С | | | 250 | | | 177.133 | -0.210 | | 11.97 | A | С |
| MOTA | 1064 | 0 | | | 250 | | | 178.286 | 0.057 | | 14.99 | A | 0 |
| ATOM | 1065 | N | | | 251 | 175.68 | 6 | 176.478 | -1.208 | 1.00 | 14.14 | A | N |
| ATOM | 1066 | CA | | | 251 | 176.69 | 0 | 177.099 | -2.079 | 1.00 | 13.45 | A | C |
| MOTA | 1067 | CB | ARG | A | 251 | 176.08 | 0 | 178.305 | -2.792 | 1.00 | 14.05 | A | С |
| MOTA | 1068 | CG | ARG | Α | 251 | 174.97 | 6 | 177.936 | -3.779 | 1.00 | 21.06 | Α | С |
| MOTA | 1069 | CD | ARG | Α | 251 | 175.44 | 1 | 178.112 | -5.227 | 1.00 | 27.95 | A | С |
| MOTA | 1070 | NE | ARG | Α | 251 | 175.54 | 7 | 176.844 | -5.943 | 1.00 | 31.22 | A. | N |
| MOTA | 1071 | CZ | ARG | Α | 251 | 176.39 | 1 | 176.615 | -6.949 | 1.00 | 31.35 | A | С |
| ATOM | 1072 | NH1 | ARG | Α | 251 | 177.21 | 4 | 177.570 | -7.368 | 1.00 | 28.63 | A | N |
| MOTA | 1073 | NH2 | ARG | Α | 251 | 176.42 | 7 | 175.422 | -7.526 | 1.00 | 31.96 | A | N |
| MOTA | 1074 | С | ARG | A | 251 | 177.97 | 4 | 177.493 | -1.362 | 1.00 | 12.30 | A | С |
| ATOM | 1075 | 0 | ARG | Α | 251 | 178.61 | 8 | 178.472 | -1.703 | 1.00 | 12.69 | A | 0 |
| ATOM | 1076 | N | VAL | Α | 252 | 178.34 | 4 | 176.714 | ~0.363 | 1.00 | 11.12 | A | N |
| ATOM | 1077 | CA | VAL | Α | 252 | 179.56 | 9 | 176.971 | 0.368 | 1.00 | 12.45 | A | С |
| MOTA | 1078 | CB | VAL | Α | 252 | 179.33 | 8 | 176.810 | 1.885 | 1.00 | 12.23 | Α | С |
| ATOM | 1079 | CG1 | VAL | A | 252 | 180.65 | 1 | 176.509 | 2.587 | 1.00 | 9.08 | A | С |
| ATOM | 1080 | CG2 | VAL | A | 252 | 178.68 | 1 | 178.059 | 2.446 | 1.00 | 10.54 | A | С |
| ATOM | 1081 | С | VAL | Α | 252 | 180.60 | 4 | 175.940 | -0.083 | 1.00 | 15.27 | Α | С |
| MOTA | 1082 | 0 | VAL | Α | 252 | 180.26 | 7 | 174.774 | -0.265 | 1.00 | 12.78 | A | 0 |
| ATOM | 1083 | N | ILE | Α | 253 | 181.84 | 0 | 176.373 | -0.326 | 1.00 | 13.72 | A | N |
| ATOM | 1084 | CA | ILE | Α | 253 | 182.87 | 2 | 175.419 | -0.680 | 1.00 | 10.89 | A | С |
| MOTA | 1085 | CB | ILE | Α | 253 | 183.67 | 0 | 175.788 | -1.957 | 1.00 | 11.67 | Α | С |
| ATOM | 1086 | CG2 | ILE | Α | 253 | 184.42 | 6 | 174.535 | -2.441 | 1.00 | 5.83 | A | С |
| ATOM | 1087 | CG1 | ILE | Α | 253 | 182.73 | 3 | 176.323 | -3.059 | 1.00 | 10.28 | A | С |
| ATOM | 1088 | CD1 | ILE | Α | 253 | 183.43 | 9 | 176.812 | -4.329 | 1.00 | 3.57 | A | С |
| MOTA | 1089 | С | ILE | Α | 253 | 183.83 | 1 | 175.453 | 0.498 | 1.00 | 13.01 | A | С |
| ATOM | 1090 | 0 | ILE | Α | 253 | 184.34 | 7 | 176.524 | 0.849 | 1.00 | 13.11 | A | 0 |
| ATOM | 1091 | N | HIS | Α | 254 | 184.05 | 0 | 174.288 | 1.113 | 1.00 | 13.19 | A | N |
| ATOM | 1092 | CA | HIS | Α | 254 | 184.94 | 3 | 174.161 | 2.259 | 1.00 | 12.95 | A | С |
| MOTA | 1093 | CB | HIS | Α | 254 | 184.86 | 8 | 172.745 | 2.843 | 1.00 | 12.70 | A | C |
| ATOM | 1094 | CG | HIS | Α | 254 | 185.58 | 7 | 172.606 | 4.160 | 1.00 | 12.92 | A | С |
| ATOM | 1095 | CD2 | HIS | A | 254 | 185.20 | 6 | 172.914 | 5.423 | 1.00 | 9.91 | A | C |
| MOTA | 1096 | ND1 | HIS | Α | 254 | 186.89 | 8 | 172.180 | 4.257 | 1.00 | 13.73 | A | N |
| ATOM | 1097 | CE1 | HIS | Α | 254 | 187.29 | 0 | 172.229 | 5.515 | 1.00 | 10.14 | A | С |
| ATOM | 1098 | NE2 | HIS | A | 254 | | | 172.671 | 6.243 | | 11.29 | A | N |
| ATOM | 1099 | С | | | 254 | | | 174.507 | 1.889 | 1.00 | 13.04 | Α | С |
| ATOM | 1100 | Ō | | | 254 | | | 175.438 | 2.447 | | 14.41 | Α | 0 |
| ATOM | 1101 | N | | | 255 | | | 173.743 | 0.953 | | 12.07 | Α | N |
| ATOM | 1102 | CA | | | 255 | | | 173.910 | 0.438 | 1.00 | 12.35 | A | C |
| ATOM | 1103 | СВ | | | 255 | | | 175.341 | -0.050 | | 13.05 | A | C |
| ATOM | 1104 | CG | | | 255 | | | 175.664 | -1.200 | | 15.96 | A | Č |
| ATOM | 1105 | CD | | | 255 | | | 176.885 | -1.997 | | 11.42 | A | č |
| ATOM | 1106 | NE | | | 255 | | | 178.075 | -1.183 | | 13.42 | A. | N |
| ATOM | 1107 | CZ | | | 255 | | | 179.295 | -1.690 | | 17.97 | A | Ċ |
| ATOM | 1108 | | ARG | | | | | 179.453 | -3.012 | | 12.59 | A | N |
| ATOM | 1100 | | ARG | | | | | 180.348 | -0.880 | | 11.08 | A | N |
| ATOM | 1110 | C | | | 255 | | | 173.491 | 1.328 | | 14.82 | A | C |
| ATOM | 1111 | 0 | | | 255 | | | 173.451 | 0.914 | | 16.45 | A | õ |
| ATOM | 1112 | N | | | 256 | | | 172.959 | 2.528 | | 13.90 | A | Ŋ |
| ATOM | 1113 | CA | | | 256 | | | 172.522 | 3.364 | | 14.13 | A | C |
| AT ON | **** | UM | MOE | - | 200 | 1,0.33 | _ | _, | 2.504 | | | •• | ~ |

| MOTA | 1114 | СВ | ASP : | A | 256 | | 173.631 | 4.341 | 1.00 15.61 | A | С |
|--------------|--------------|-----------|------------|---|------------|---------|------------------------|------------------|--------------------------|--------|--------|
| MOTA | 1115 | CG | ASP . | | | | 173.408 | 4.930 | 1.00 17.71 | A | C |
| MOTA | 1116 | | ASP . | | | | 172.950 | 4.217 | 1.00 18.23 | A | 0 |
| MOTA | 1117 | | ASP . | | | | 173.712 | 6.130 | 1.00 20.01 | A | 0 C |
| ATOM | 1118 | C | ASP | | | | 171.231 | 4.094 | 1.00 14.83 1.00 17.90 | A A | 0 |
| ATOM | 1119 | 0 | ASP . | | | | 171.088 | 5.300 3.321 | 1.00 17.90 | A | И |
| MOTA | 1120 | N | ILE . | | | | 170.285 168.978 | 3.809 | 1.00 14.83 | A | C |
| MOTA | 1121 | CA CB | ILE | | | | 168.318 | 2.821 | 1.00 16.68 | A | Č |
| ATOM ATOM | 1122 1123 | | ILE | | | | 166.834 | 3.106 | 1.00 18.21 | A | č |
| MOTA | 1124 | CG1 | | | | | 169.010 | 2.909 | 1.00 19.11 | A | Ċ |
| ATOM | 1125 | | ILE | | | | 168.636 | 1.771 | 1.00 26.98 | A | С |
| MOTA | 1126 | C | ILE | | | | 168.170 | 3.888 | 1.00 16.84 | A | С |
| ATOM | 1127 | 0 | ILE | A | 257 | 191.180 | 168.019 | 2.890 | 1.00 19.23 | A | 0 |
| MOTA | 1128 | N | LYS | Α | 258 | | 167.673 | 5.079 | 1.00 14.42 | A | N |
| ATOM | 1129 | CA | LYS | | | | 166.861 | 5.321 | 1.00 13.61 | A | C |
| MOTA | 1130 | CB | LYS | | | | 167.696 | 5.165 | 1.00 11.12 | A | C |
| ATOM | 1131 | CG | LYS | | | | 168.912 | 6.021 | 1.00 10.35 | A | C |
| MOTA | 1132 | CD | LYS | | | | 169.397 | 5.941 | 1.00 11.98 1.00 10.31 | A A | C |
| MOTA | 1133 | CE | LYS LYS | | | | 170.539 171.028 | 6.844 6.523 | 1.00 10.31 | A | Ŋ |
| MOTA | 1134 1135 | NZ C | LYS | | | | 166.275 | 6.728 | 1.00 13.12 | A | C |
| ATOM ATOM | 1136 | 0 | LYS | | | | 166.807 | 7.565 | 1.00 12.94 | A | ō |
| MOTA | 1137 | N | PRO | | | | 165.180 | 7.011 | 1.00 13.48 | A | N |
| ATOM | 1138 | CD | PRO | | | | 164.582 | 6.181 | 1.00 11.93 | A | С |
| MOTA | 1139 | CA | PRO | Α | 259 | 192.487 | 164.525 | 8.329 | 1.00 14.07 | A | С |
| ATOM | 1140 | CB | PRO | A | 259 | 193.641 | 163.517 | 8.267 | 1.00 14.89 | A | С |
| ATOM | 1141 | CG | | | 259 | | 163.197 | 6.778 | 1.00 14.98 | A | C |
| ATOM | 1142 | C | | | 259 | | 165.413 | 9.583 | 1.00 15.36 | A | C |
| MOTA | 1143 | 0 | | | 259 | | 165.171 | 10.520 | 1.00 15.88 | A | 0 |
| ATOM | 1144 | N | | | 260 | | 166.428 | 9.593 10.734 | 1.00 15.22 1.00 19.96 | A A | И С |
| MOTA | 1145 1146 | CA CB | | | 260 260 | | 167.340 168.225 | 10.754 | 1.00 19.90 | A | |
| ATOM ATOM | 1147 | CG | | | 260 | | 167.457 | 10.516 | 1.00 29.11 | A | |
| ATOM | 1148 | CD | | | 260 | | 167.140 | 9.092 | 1.00 32.88 | A | |
| ATOM | 1149 | | GLU | | | | 5 166.656 | 8.235 | 1.00 33.12 | A | 0 |
| ATOM | 1150 | OE2 | | | 260 | 197.823 | 3 167.360 | 8.841 | 1.00 35.49 | A | |
| ATOM | 1151 | С | GLU | A | 260 | | 168.252 | 10.924 | 1.00 18.80 | A | C |
| MOTA | 1152 | 0 | | | 260 | | 168.905 | 11.957 | 1.00 18.71 | A | |
| ATOM | 1153 | N | | | 261 | | 168.309 | 9.922 | 1.00 16.14 | A | |
| MOTA | 1154 | CA | | | 261 | | 169.139 | 10.014 | 1.00 14.12 1.00 12.74 | A A | |
| ATOM | 1155 | CB | | | 261 261 | | 170.036 171.176 | 8.799 8.824 | 1.00 12.74 | A | C |
| ATOM ATOM | 1156 1157 | CG OD1 | ASN | | | | 9 171.446 | 9.840 | 1.00 12.57 | A | |
| ATOM | 1158 | | ASN | | | | 3 171.868 | 7.705 | 1.00 11.18 | A | |
| ATOM | 1159 | | | | 261 | | 168.329 | | 1.00 14.87 | A | С |
| ATOM | 1160 | Ō | | | 261 | | 4 168.855 | 10.027 | 1.00 14.12 | A | 0 |
| ATOM | 1161 | N | LEU | A | 262 | 189.11 | 7 167.037 | 10.428 | 1.00 16.20 | A | |
| ATOM | 1162 | CA | | | 262 | | 6 166.127 | 10.596 | 1.00 13.58 | A | |
| ATOM | 1163 | CB | | | 262 | | 3 164.954 | 9.627 | 1.00 13.22 | A | |
| ATOM | 1164 | CG | | | 262 | | 4 165.406 | 8.162 | 1.00 15.01 1.00 8.10 | A | |
| MOTA | 1165 | | LEU LEU | | | | 2 164.230 7 166.049 | 7.232 7.834 | 1.00 10.56 | A A | |
| ATOM | 1166 1167 | CDZ | | | 262 | | 7 165.633 | 12.031 | 1.00 15.43 | A | |
| MOTA MOTA | 1168 | Ö | | | 262 | | 9 165.008 | 12.459 | 1.00 17.59 | A | |
| MOTA | 1169 | N | | | 263 | | 8 165.915 | 12.777 | 1.00 11.89 | A | |
| ATOM | 1170 | CA | | | 263 | | 6 165.505 | 14.154 | 1.00 10.46 | A | С |
| ATOM | 1171 | CB | LEU | A | 263 | | 7 166.725 | 15.005 | 1.00 13.46 | Α | |
| MOTA | 1172 | CG | LEU | A | 263 | | 4 167.921 | 14.699 | 1.00 14.28 | A | |
| ATOM | 1173 | | L LEU | | | | 8 169.055 | 15.634 | 1.00 15.02 | A | |
| MOTA | 1174 | | LEU | | | | 0 167.563 | 14.865 | 1.00 12.28 | A | |
| ATOM | 1175 | С | | | 263 | | 5 164.407 | 14.409 | 1.00 12.75 | A | C |
| MOTA | 1176 | 0 | | | 263 | | 8 164.112 9 163.780 | 13.553 15.576 | 1.00 13.83 1.00 13.44 | A A | |
| ATOM | 1177 | N | | | 264 | | 6 162.693 | 15.576 | 1.00 15.44 | A | |
| ATOM ATOM | 1178 1179 | CA CB | | | 264 | | 6 161.421 | 16.298 | 1.00 15.00 | A | |
| ATOM | 1180 | CG | | | 264 | | 8 160.821 | 15.263 | 1.00 16.94 | A | |
| ATOM | 1181 | | L LEU | | | | 3 159.499 | 15.783 | 1.00 20.04 | A | С |
| MOTA | 1182 | | LEU | | | 186.04 | 3 160.590 | 13.944 | 1.00 16.69 | A | С |
| ATOM | 1183 | C | | | 264 | 184.19 | 0 163.103 | 17.078 | 1.00 14.83 | A | С |
| | | | | | | | | | | | |

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| MOTA | 1184 | 0 | LEU | Α | 264 | 184.66 | 9 163.613 | 18.096 | 1.00 | 13.07 | | A | 0 |
|------|------|-----|-------|---|-------|---------|-----------|--------|------|-------|---|----------|---|
| ATOM | 1185 | N | GLY | Α | 265 | | 162.881 | 16.907 | | 14.85 | | A | N |
| MOTA | 1186 | CA | | | 265 | | 3 163.218 | 17.947 | | 15.69 | | A | C |
| ATOM | 1187 | C | | | 265 | | 162.127 | 18.999 | | | | | |
| ATOM | 1188 | Õ | | | 265 | | 7 161.144 | | | 17.48 | | A | С |
| ATOM | 1189 | | | | | | | 18.989 | | 19.40 | | A | 0 |
| | | N | | | 266 | | 162.306 | 19.899 | | 17.64 | | A | N |
| ATOM | 1190 | CA | | | 266 | _ | 161.398 | 21.007 | 1.00 | 18.83 | | Α | С |
| MOTA | 1191 | CB | | | 266 | | 7 161.895 | 21.766 | 1.00 | 17.49 | | A | С |
| MOTA | 1192 | OG | SER | Α | 266 | | 7 161.294 | 23.037 | 1.00 | 31.06 | | Α | 0 |
| ATOM | 1193 | С | SER | Α | 266 | 180.45 | 7 159.923 | 20.615 | 1.00 | 16.59 | | Α | C |
| MOTA | 1194 | 0 | SER | Α | 266 | 180.77 | 159.025 | 21.389 | | 16.64 | | Α | 0 |
| ATOM | 1195 | N | ALA | A | 267 | 179.966 | 159.675 | 19.412 | | 15.97 | | A | N |
| MOTA | 1196 | CA | ALA | Α | 267 | 179.73 | 1 158.314 | 18.939 | | 17.67 | | A | c |
| ATOM | 1197 | CB | ALA | А | 267 | | 3 158.163 | 18.456 | | 14.65 | | A | c |
| ATOM | 1198 | C | | | 267 | | 157.930 | 17.815 | | 18.92 | | | |
| ATOM | 1199 | ō | | | 267 | | 3 157.040 | 17.025 | | | | A | C |
| MOTA | 1200 | N | | | 268 | | 2 158.604 | | | 21.00 | | A | 0 |
| ATOM | 1201 | CA | | | 268 | | | 17.716 | | 21.24 | | A | N |
| ATOM | 1201 | | | | | | 1 158.278 | 16.648 | | 22.38 | | A | С |
| | | C | | | 268 | | 9 158.773 | 15.282 | | 21.15 | | Α | С |
| ATOM | 1203 | 0 | | | 268 | | 9 158.323 | 14.266 | 1.00 | 20.78 | | A | 0 |
| ATOM | 1204 | N | | | 269 | | 4 159.690 | 15.249 | 1.00 | 19.71 | | Α | N |
| ATOM | 1205 | CA | | | 269 | | 160.239 | 13.983 | 1.00 | 18.83 | | A | C |
| ATOM | 1206 | CB | | | 269 | | 5 160.746 | 14.107 | 1.00 | 20.11 | | A | С |
| MOTA | 1207 | CG | GLU | Α | 269 | 179.23 | 9 162.020 | 14.944 | 1.00 | 27.28 | | A | C |
| MOTA | 1208 | CD | GLU | Α | 269 | 178.87 | 4 161.722 | 16.385 | 1.00 | 29.04 | | A | С |
| ATOM | 1209 | OE1 | GLU | Α | 269 | 179.762 | 2 161.324 | 17.177 | | 30.97 | | A | ō |
| ATOM | 1210 | OE2 | GLU | Α | 269 | | 7 161.868 | 16.711 | | 33.63 | | A | ŏ |
| MOTA | 1211 | С | | | 269 | | 2 161.409 | 13.549 | | 17.27 | | A | c |
| ATOM | 1212 | 0 | | | 269 | | 3 162.249 | 14.368 | | 15.38 | | A | ő |
| ATOM | 1213 | N | | | 270 | | 161.461 | 12.253 | | 14.97 | | | |
| ATOM | 1214 | CA | | | 270 | | 2 162.515 | 11.689 | | 15.39 | | A | N |
| ATOM | 1215 | CB | | | 270 | | 9 162.167 | 10.229 | | | | A | C |
| ATOM | 1216 | CG | | | 270 | | 163.071 | | | 21.78 | | A | C |
| ATOM | 1217 | | LEU | | | | | 9.408 | | 22.18 | | A | С |
| | | | | | | | 162.839 | 9.938 | | 26.73 | | A | С |
| ATOM | 1218 | | LEU | | | | 162.725 | 7.944 | | 27.39 | | A | С |
| ATOM | 1219 | С | | | 270 | | 163.876 | 11.722 | | 13.13 | | A | C |
| ATOM | 1220 | 0 | | | 270 | | 2 163.973 | 11.490 | 1.00 | 12.45 | | A | 0 |
| ATOM | 1221 | N | | | 271 | | 5 164.918 | 12.027 | 1.00 | 13.69 | | A | N |
| MOTA | 1222 | CA | | | 271 | | 166.296 | 12.025 | 1.00 | 13.80 | | A | С |
| MOTA | 1223 | CB | LYS | A | 271 | | 166.814 | 13.450 | 1.00 | 13.22 | | A | С |
| MOTA | 1224 | CG | LYS | A | 271 | 180.846 | 5 166.378 | 14.025 | 1.00 | 16.86 | | A | С |
| ATOM | 1225 | CD | LYS | A | 271 | 180.790 | 166.428 | 15.509 | 1.00 | 17.04 | | A | С |
| MOTA | 1226 | CE | LYS | A | 271 | 179.494 | 165.823 | 15.967 | 1.00 | 15.79 | | A | C |
| ATOM | 1227 | NZ | LYS | Α | 271 | 178.379 | 166.692 | 15.545 | 1.00 | 20.81 | | A | N |
| MOTA | 1228 | C | LYS | A | 271 | 183.392 | 2 167.151 | 11.270 | | 15.22 | | A | c |
| MOTA | 1229 | 0 | LYS | Α | 271 | | 6 167.152 | 11.582 | | 16.95 | | A | ő |
| MOTA | 1230 | N | ILE | Α | 272 | | 167.842 | 10.238 | | 15.55 | | A | |
| ATOM | 1231 | CA | | | 272 | | 168.702 | 9.462 | | 15.61 | | A. | N |
| ATOM | 1232 | CB | | | 272 | | 169.220 | 8.163 | | 19.61 | | A. | C |
| MOTA | 1233 | | ILE | | | | 170.269 | 7.530 | | 18.20 | | | C |
| ATOM | 1234 | | ILE | | | | 168.069 | 7.203 | | 22.81 | | A | C |
| ATOM | 1235 | | ILE | | | | 168.504 | 5.967 | | 25.62 | | A. | C |
| ATOM | 1236 | C | | | 272 | | . 169.926 | 10.303 | | | | A. | С |
| MOTA | 1237 | õ | | | 272 | | | | | 13.27 | | A. | С |
| ATOM | 1238 | | ALA | | | | 170.422 | 10.945 | | 12.04 | | A. | 0 |
| | | N | | | | | 170.428 | 10.294 | | 11.17 | | A | N |
| ATOM | 1239 | CA | ALA | | | | 171.623 | 11.069 | | 13.73 | | A | С |
| ATOM | 1240 | CB | | | 273 | | 171.248 | 12.376 | 1.00 | 10.14 | | A | С |
| MOTA | 1241 | С | ALA | | | | 172.498 | 10.225 | | 16.38 | | A | С |
| MOTA | 1242 | 0 | ALA | | | | 172.208 | 9.047 | 1.00 | 16.96 | | A | 0 |
| ATOM | 1243 | N | ASP | | | | 173.568 | 10.834 | 1.00 | 17.04 | i | A | N |
| MOTA | 1244 | CA | ASP | | | | 174.500 | 10.200 | 1.00 | | 1 | Ą | C |
| ATOM | 1245 | CB | ASP | | | 189.288 | 173.805 | 10.074 | 1.00 | 17.02 | | Ą | Ċ |
| ATOM | 1246 | CG | ASP | A | 274 | | 174.786 | 9.800 | 1.00 | | | Ā | č |
| MOTA | 1247 | OD1 | ASP | Α | 274 | | 175.999 | 9.635 | 1.00 | | | Ā | ŏ |
| MOTA | 1248 | OD2 | ASP | Α | 274 | | 174.338 | 9.753 | 1.00 | | | À | ŏ |
| ATOM | 1249 | C | ASP | | | | 175.064 | 8.838 | 1.00 | | | 4 | C |
| ATOM | 1250 | ō | ASP | | | | 174.604 | 7.776 | 1.00 | | | | |
| ATOM | 1251 | N | PHE | | | | 176.065 | 8.881 | 1.00 | | | <i>Y</i> | 0 |
| ATOM | 1252 | CA | PHE | | | | 176.688 | 7.666 | 1.00 | | | <i>,</i> | N |
| ATOM | 1253 | CB | PHE | | | | 177.108 | | | | | A | C |
| 011 | | CD | r 116 | ~ | - 1 - | 104.002 | T11.T00 | 7.835 | 1.00 | 13.16 | 1 | A. | С |

| MOTA | 1254 | CG | PHE | Α | 275 | 183.640 | 175.948 | 7.721 | 1.00 12.72 | | A | С |
|------|------|-----|-----|----|-----|---------|-----------|--------|------------|-----|-----|---|
| ATOM | 1255 | | PHE | | | | 174.994 | | | | | |
| | | | | | | | | 8.746 | 1.00 11.42 | | A. | С |
| ATOM | 1256 | | PHE | | | | 175.727 | 6.535 | 1.00 11.44 | | A | С |
| MOTA | 1257 | CE1 | PHE | Α | 275 | 182.768 | 173.843 | 8.581 | 1.00 10 04 | | A | С |
| MOTA | 1258 | CE2 | PHE | Α | 275 | 182,157 | 174.568 | 6.367 | 1.00 12.57 | | A | С |
| ATOM | 1259 | CZ | | | 275 | | 173.631 | 7.396 | 1.00 11.15 | | | |
| | | | | | | | | | | | A. | C |
| ATOM | 1260 | С | | | 275 | | 177.868 | 7.289 | 1.00 15.87 | | A : | С |
| ATOM | 1261 | 0 | PHE | A | 275 | 186.541 | . 178.780 | 6.568 | 1.00 15.07 | | A | 0 |
| MOTA | 1262 | N | GLY | Α | 276 | 188.221 | 177.820 | 7.751 | 1.00 15.09 | | A | N |
| MOTA | 1263 | CA | | | 276 | | 178.875 | | | | | |
| | | | | | | | | 7.452 | 1.00 17.20 | | A | C |
| ATOM | 1264 | С | | | 276 | 189.322 | 179.285 | 5.983 | 1.00 16.44 | | A. | С |
| ATOM | 1265 | 0 | GLY | A | 276 | 189.368 | 180.482 | 5.665 | 1.00 17.13 | | A | 0 |
| MOTA | 1266 | N | TRP | Α | 277 | 189.378 | 178.307 | 5.082 | 1.00 13.73 | | Ą | N |
| ATOM | 1267 | CA | | | 277 | | 178.596 | 3.664 | | | | |
| | | | | | | | | | 1.00 14.40 | | A. | C |
| ATOM | 1268 | CB | | | 277 | | 177.667 | 3.071 | 1.00 20.13 | | A. | С |
| ATOM | 1269 | CG | | | 277 | 191.860 | 177.753 | 3.789 | 1.00 22.40 | | A. | С |
| ATOM | 1270 | CD2 | TRP | Α | 277 | 192.691 | . 178.904 | 3.893 | 1.00 23.73 | | A. | С |
| ATOM | 1271 | | TRP | | | | 178.558 | 4.701 | 1.00 26.05 | | | |
| ATOM | 1272 | | TRP | | | | | | | | A. | C |
| | | | | | | | 180.198 | 3.375 | 1.00 25.94 | | A. | С |
| MOTA | 1273 | | TRP | | | | 176.777 | 4.517 | 1.00 23.25 | 7 | A. | С |
| ATOM | 1274 | | TRP | | | 193.625 | 177.250 | 5.074 | 1.00 24.53 | | A. | N |
| ATOM | 1275 | CZ2 | TRP | Α | 277 | | 179.467 | 5.015 | 1.00 27.86 | | A. | C |
| ATOM | 1276 | | TRP | | | | 181.106 | | | | | |
| | | | | | | | | | 1.00 28.74 | | A | С |
| MOTA | 1277 | | TRP | | | | . 180.733 | 4.496 | 1.00 26.68 | 1 | A. | С |
| ATOM | 1278 | С | TRP | A | 277 | 188.202 | 178.467 | 2.888 | 1.00 13.46 | | A | С |
| MOTA | 1279 | 0 | TRP | Α | 277 | 188.190 | 178.362 | 1.664 | 1.00 14.44 | | A | 0 |
| ATOM | 1280 | N | | | 278 | | 178.481 | 3.605 | 1.00 14.67 | | | |
| MOTA | 1281 | CA | | | 278 | | | | | | A | N |
| | | | | | | | 178.360 | 2.973 | 1.00 16.81 | i i | A | С |
| ATOM | 1282 | CB | | | 278 | 184.785 | 177.937 | 4.009 | 1.00 18.65 | 7 | A. | С |
| ATOM | 1283 | OG | SER | A | 278 | 185.042 | 176.588 | 4.334 | 1.00 31.56 | 7 | Ą | 0 |
| MOTA | 1284 | С | SER | Α | 278 | 185.338 | 179.620 | 2.269 | 1.00 15.59 | | Ą | Č |
| ATOM | 1285 | o | | | 278 | | 180.700 | | | | | |
| | | | | | | | | 2.456 | 1.00 13.40 | | A | 0 |
| ATOM | 1286 | N | | | 279 | | 179.468 | 1.427 | 1.00 12.47 | 2 | A. | N |
| ATOM | 1287 | CA | | | 279 | 183.790 | 180.622 | 0.750 | 1.00 15.04 | 2 | A | С |
| MOTA | 1288 | CB | VAL | A. | 279 | 184.631 | 181.010 | -0.524 | 1.00 14.76 | 7 | A | С |
| ATOM | 1289 | CG1 | VAL | | | 184.436 | 179.985 | -1.646 | 1.00 10.49 | | | č |
| ATOM | 1290 | | VAL | | | | 182.419 | | | | A | |
| | | | | | | | | -0.971 | 1.00 9.51 | I | A | С |
| ATOM | 1291 | C | | | 279 | | 180.399 | 0.352 | 1.00 15.66 | 7 | A. | С |
| MOTA | 1292 | 0 | VAL | Α | 279 | 181.902 | 179.259 | 0.162 | 1.00 16.74 | 1 | P. | 0 |
| ATOM | 1293 | N | HIS | Α | 280 | 181.604 | 181.491 | 0.276 | 1.00 14.84 | 7 | A. | N |
| ATOM | 1294 | CA | HIS | Α | 280 | | 181.389 | -0.133 | 1.00 17.48 | | Ä | |
| MOTA | 1295 | CB | | | 280 | | 182.330 | 0.694 | | | | C |
| | 1296 | | | | | | | | 1.00 14.36 | | 7 | С |
| ATOM | | CG | | | 280 | | 182.230 | 0.336 | 1.00 16.95 | Į | 4 | С |
| ATOM | 1297 | | HIS | | | 177.154 | 181.176 | -0.102 | 1.00 16.10 | 7 | A. | С |
| ATOM | 1298 | ND1 | HIS | Α | 280 | 177.045 | 183.323 | 0.300 | 1.00 15.76 | 1 | A. | N |
| MOTA | 1299 | CE1 | HIS | Α | 280 | 175.864 | 182.946 | -0.154 | 1.00 17.22 | I | | Ċ |
| ATOM | 1300 | | HIS | | | | 181.648 | | 1.00 18.56 | | | |
| ATOM | 1301 | | | | | | | | | | A. | N |
| | | C | | | 280 | | 181.772 | -1.622 | 1.00 17.74 | P | 4 | C |
| ATOM | 1302 | 0 | | | 280 | 180.439 | 182.942 | -1.989 | 1.00 16.22 | F | 4 | 0 |
| MOTA | 1303 | N | | | 281 | 180.048 | 180.773 | -2.480 | 1.00 15.79 | P | 1 | N |
| MOTA | 1304 | CA | ALA | Α | 281 | 180.066 | 180.984 | -3.930 | 1.00 17.35 | | Ā | c |
| ATOM | 1305 | CB | ALA | | | | 180.047 | -4.565 | 1.00 15.43 | | | |
| ATOM | 1306 | c | | | 281 | | | | | P | | С |
| | | | | | | | 180.779 | -4.610 | 1.00 18.31 | P | 1 | С |
| MOTA | 1307 | 0 | ALA | | | | 179.809 | -5.311 | 1.00 18.09 | P | 1 | 0 |
| ATOM | 1308 | N | PRO | Α | 282 | 177.754 | 181.726 | -4.412 | 1.00 20.27 | 2 | 1 | N |
| ATOM | 1309 | CD | PRO | Α | 282 | 177.983 | 182.946 | -3.597 | 1.00 20.44 | Þ | | Ĉ |
| ATOM | 1310 | CA | PRO | А | 282 | | 181.701 | -4.974 | 1.00 21.92 | | | |
| ATOM | 1311 | CB | | | | | | | | A | | С |
| | | | | | 282 | | 183.032 | -4.483 | 1.00 21.47 | Z | | C |
| ATOM | 1312 | CG | PRO | | | | 183.413 | -3.327 | 1.00 21.85 | P | | С |
| ATOM | 1313 | С | PRO | Α | 282 | 176.326 | 181.581 | -6.480 | 1.00 22.24 | A | | С |
| MOTA | 1314 | 0 | PRO | A | 282 | 175.611 | 180.729 | -6.987 | 1.00 24.89 | A | | ō |
| ATOM | 1315 | N | SER | | | | 182.439 | -7.163 | 1.00 24.90 | | | |
| ATOM | 1316 | CA | SER | | | | 182.464 | | | A | | N |
| | | | | | | | | -8.629 | 1.00 28.30 | A | | С |
| ATOM | 1317 | CB | SER | | | | 183.837 | -9.202 | 1.00 26.31 | A | | С |
| ATOM | 1318 | OG | SER | A | 283 | 175.659 | 184.461 | -8.492 | 1.00 30.72 | A | | 0 |
| ATOM | 1319 | С | SER | A | 283 | 178.454 | 182.133 | -9.327 | 1.00 27.14 | A | | č |
| ATOM | 1320 | 0 | SER | | | | | | 1.00 31.35 | | | |
| ATOM | 1321 | N | SER | | | | 183.011 | | | A | | 0 |
| | | | | | | | | -9.147 | 1.00 25.92 | A | | N |
| MOTA | 1322 | CA | SER | | | | 182.937 | -9.789 | 1.00 26.41 | A | | С |
| ATOM | 1323 | CB | SER | Α | 284 | 181.476 | 184.252 | -9.583 | 1.00 26.11 | А | | С |
| | | | | | | | | | | | | - |

| ATOM | 1324 | OG | SER . | A | 284 | 180.590 | 185.288 | -9.231 | 1.00 | 32.06 | Į | A | 0 |
|--------------|--------------|-----|------------|---|-----|---------|------------------------|---------|------|----------------|-----|--------|--------|
| MOTA | 1325 | С | SER . | A | 284 | 181.720 | 181.869 | -9.346 | | 24.70 | 1 | A. | С |
| ATOM | 1326 | 0 | SER | A | 284 | 181.617 | 181.347 | -8.254 | 1.00 | 26.06 | 1 | A | 0 |
| ATOM | 1327 | N | ARG | Α | 285 | 182.717 | 181.636 | -10.192 | 1.00 | 23.60 | 2 | Į. | N |
| ATOM | 1328 | CA | ARG | A | 285 | 183.782 | 180.701 | -9.910 | 1.00 | 25.00 | 1 | A. | С |
| MOTA | 1329 | CB | ARG | Α | 285 | 184.337 | 180.169 | -11.225 | 1.00 | 25.95 | 2 | A. | C |
| ATOM | 1330 | CG | ARG | A | 285 | 183.367 | 179.201 | -11.935 | 1.00 | 31.00 | 2 | ¥. | С |
| ATOM | 1331 | CD | ARG | A | 285 | 184.154 | 178.152 | -12.746 | 1.00 | 38.12 | 1 | A. | С |
| ATOM | 1332 | NE | ARG | A | 285 | 184.419 | 178.543 | -14.135 | 1.00 | 42.96 | 1 | 4 | N |
| MOTA | 1333 | CZ | ARG | Α | 285 | 185.202 | 177.856 | -14.971 | 1.00 | 45.91 | 7 | A. | С |
| ATOM | 1334 | NH1 | ARG | A | 285 | | 176.744 | | 1.00 | 46.53 | 1 | A. | N |
| ATOM | 1335 | NH2 | ARG | Α | 285 | 185.364 | 178.267 | -16.225 | 1.00 | 46.52 | 1 | 4 | N |
| ATOM | 1336 | С | ARG | | | | 181.436 | -9.074 | 1.00 | 23.19 | 1 | A | С |
| MOTA | 1337 | 0 | ARG | Α | 285 | 184.791 | 182.652 | -8.873 | 1.00 | 23.63 | 1 | A | 0 |
| ATOM | 1338 | N | ARG | Α | 286 | 185.871 | 180.720 | -8.578 | 1.00 | 22.25 | i | A | N |
| ATOM | 1339 | CA | ARG | А | 286 | 186.898 | 181.369 | -7.770 | 1.00 | 18.11 | i | A | С |
| MOTA | 1340 | CB | ARG | Α | 286 | 186.781 | 180.826 | -6.344 | 1.00 | 16.41 | 7 | Ą | С |
| MOTA | 1341 | CG | ARG | Α | 286 | 185.467 | 181.252 | -5.671 | 1.00 | 17.03 | į. | A | С |
| MOTA | 1342 | CD | ARG | Α | 286 | 185.642 | 182.655 | -5.179 | 1.00 | 16.99 | 7 | A | C |
| MOTA | 1343 | NE | ARG | Α | 286 | 184.443 | 183.221 | -4.632 | 1.00 | 25.38 | | A | N |
| MOTA | 1344 | CZ | ARG | Α | 286 | 184.398 | 184.417 | -4.072 | 1.00 | 26.94 | 1 | A | С |
| MOTA | 1345 | NH1 | ARG | Α | 286 | 185.509 | 185.138 | -3.995 | 1.00 | 28.48 | | A | N |
| ATOM | 1346 | NH2 | ARG | A | 286 | 183.244 | 184.894 | -3.605 | 1.00 | 30.62 | 7 | A | N |
| ATOM | 1347 | С | ARG | А | 286 | 188.309 | 181.189 | -8.339 | 1.00 | 19.47 | 7 | A. | С |
| MOTA | 1348 | 0 | ARG | Α | 286 | 188.537 | 180.305 | -9.174 | 1.00 | 17.62 | 1 | Ą | 0 |
| ATOM | 1349 | N | TPO | Α | 287 | 189.226 | 182.041 | -7.916 | 1.00 | 21.77 | | A | N |
| MOTA | 1350 | ÇA | TPO | Α | 287 | 190.558 | 181.974 | -8.377 | | 21.28 | , i | A | С |
| MOTA | 1351 | CB | TPO | Α | 287 | | 183.306 | | | 25.22 | | A | С |
| MOTA | 1352 | CG2 | TPO | Α | 287 | | 183.372 | -10.421 | | 22.17 | | A | С |
| ATOM | 1353 | OG1 | TPO | Α | 287 | 190.484 | 184.557 | -8.448 | | 33.29 | | A | 0 |
| MOTA | 1354 | P | | | 287 | | 2 185.763 | | | 33.70 | | A | P |
| MOTA | 1355 | | TPO | | | | 2 186.991 | | | 41.17 | | A | 0 |
| ATOM | 1356 | | TPO | | | | 185.199 | | | 37.62 | | A. | 0 |
| MOTA | 1357 | | TPO | | | | 186.067 | | | 41.70 | | A. | 0 |
| ATOM | 1358 | С | | | 287 | | 2 181.717 | | | 16.99 | | A. | C |
| MOTA | 1359 | 0 | | | 287 | | 5 181.536 | | | 25.86 | | A. | 0 |
| MOTA | 1360 | N | | | 288 | | 181.614 | | | 16.91 | | A | N |
| ATOM | 1361 | CA | | | 288 | | 5 181.441 | | 1.00 | 16.31 | | A | C |
| ATOM | 1362 | CB | | | 288 | | 2 181.750 | | | 18.77 | | A. | C |
| MOTA | 1363 | | TPO | | | | 181.949 | | | 16.50 | | A. | C |
| ATOM | 1364 | OG1 | | | | | 183.015 | | | 23.64 | | A. | O P |
| ATOM | 1365 | P | | | 288 | | 3 183.188 4 182.723 | | | 18.56 19.25 | | A A | 0 |
| ATOM | 1366 1367 | | TPO TPO | | | | 7 182.723 | | | 24.67 | | A. | 0 |
| ATOM | 1368 | | TPO | | | | 184.760 | | 1.00 | 24.29 | | A. | ŏ |
| ATOM ATOM | 1369 | C | | | 288 | | 180.109 | | | 17.62 | | A | c |
| | 1370 | Ö | | | 288 | | 178.986 | | | 16.48 | | A | ŏ |
| MOTA MOTA | 1371 | N | | | 289 | 194.15 | 2 180.122 | -4.825 | | 19.62 | | A | N |
| ATOM | 1372 | CA | | | 289 | | 3 178.875 | | | 20.29 | | A | C |
| ATOM | 1373 | CB | | | 289 | | 9 178.759 | | | 21.71 | | A. | c |
| MOTA | 1374 | CG | | | 289 | | 7 177.458 | | | 25.59 | | A | C |
| ATOM | 1375 | | LEU | | | | 5 176.298 | | | 30.17 | | A | С |
| ATOM | 1376 | | LEU | | | | 5 177.596 | | 1.00 | 26.69 | | A | С |
| ATOM | 1377 | С | LEU | Α | 289 | 194.83 | 3 178.800 | -2.900 | 1.00 | 17.60 | | A | С |
| MOTA | 1378 | 0 | LEU | Α | 289 | | 3 179.646 | | 1.00 | 20.61 | | A | 0 |
| ATOM | 1379 | N | CYS | Α | 290 | 194.19 | 1 177.810 | -2.307 | 1.00 | 16.97 | | A | N |
| MOTA | 1380 | CA | CYS | Α | 290 | 194.20 | 4 177.679 | -0.844 | 1.00 | 18.91 | | A | С |
| MOTA | 1381 | CB | CYS | Α | 290 | 193.10 | 2 178.535 | -0.201 | 1.00 | 16.86 | , | A | С |
| ATOM | 1382 | SG | CYS | Α | 290 | | 4 178.234 | | 1.00 | 22.10 | | A | s |
| MOTA | 1383 | С | CYS | A | 290 | | 3 176.211 | | | 17.81 | | A | С |
| ATOM | 1384 | 0 | CYS | A | 290 | 193.55 | 4 175.403 | | 1.00 | 15.28 | | A | 0 |
| MOTA | 1385 | N | | | 291 | | 0 175.862 | | | 19.11 | | A | N |
| MOTA | 1386 | CA | | | 291 | | 3 174.484 | | 1.00 | 18.98 | | A | С |
| ATOM | 1387 | С | | | 291 | | 6 173.896 | | | 19.71 | | A | С |
| ATOM | 1388 | 0 | | | 291 | | 8 174.606 | | | 21.01 | | A | 0 |
| MOTA | 1389 | N | | | 292 | | 6 172.584 | | | 18.60 | | A | N |
| MOTA | 1390 | CA | | | 292 | | 171.837 | | | 16.87 | | A | C |
| ATOM | 1391 | CB | | | 292 | | 8 170.657 | | | 19.75 | | A | С |
| MOTA | 1392 | | THR | | | | 7 171.126 | | | 25.57 | | A | 0 |
| MOTA | 1393 | CG2 | THR | A | 292 | 197.56 | 3 169.991 | 3.407 | 1.00 | 18.64 | | A | С |

| ATOM | 1394 | С | THR A | 292 | 197.453 | 171.308 | 0.652 | 1.00 | 17.38 | A | С |
|--------------|--------------|----------|----------------|-------|---------|------------------------|-------------------|------|----------------|--------|---|
| ATOM | 1395 | 0 | THR A | | 196.772 | 170.864 | -0.269 | 1.00 | 16.20 | A | 0 |
| MOTA | 1396 | N | LEU A | 293 | 198.780 | 171.347 | 0.631 | 1.00 | 18.38 | A | N |
| ATOM | 1397 | CA | LEU A | | | 170.868 | -0.511 | 1.00 | | A | C |
| MOTA | 1398 | CB | LEU A | | | 170.747 | -0.102 | 1.00 | | A | C |
| MOTA | 1399 | CG | LEU A | | | 170.217 | -1.188 | 1.00 | | A | C |
| MOTA | 1400 | | LEU A | | | 171.229 | -2.316 | 1.00 | | A | C |
| ATOM | 1401 | | LEU A | | | 169.962 169.533 | -0.603 -1.126 | 1.00 | | A A | C |
| MOTA | 1402 1403 | 0 | LEU A | | | 169.496 | -2.287 | 1.00 | | Ā | ő |
| MOTA MOTA | 1403 | И | ASP A | | | 168.447 | -0.355 | 1.00 | _ | A | Ŋ |
| ATOM | 1405 | CA | ASP A | | | 167.143 | -0.868 | 1.00 | | A | c |
| ATOM | 1406 | CB | ASP A | | | 166.048 | 0.164 | 1.00 | | A | С |
| MOTA | 1407 | CG | ASP A | | 200.527 | 165.669 | 0.175 | 1.00 | 23.92 | А | С |
| MOTA | 1408 | OD1 | ASP A | 294 | 201.065 | 165.254 | -0.891 | 1.00 | 23.94 | Α | 0 |
| ATOM | 1409 | OD2 | ASP A | 294 | | 165.783 | 1.245 | 1.00 | | A | |
| ATOM | 1410 | С | ASP A | | | 167.026 | -1.309 | 1.00 | | A | C |
| MOTA | 1411 | 0 | ASP A | | | 166.084 | -2.011 | 1.00 | | A | |
| ATOM | 1412 | N | TYR A | | | 167.996 | -0.923 | 1.00 | | A | |
| ATOM | 1413 | CA | TYR A | | | 167.963 | -1.267 -0.001 | 1.00 | 12.35 | A A | |
| ATOM ATOM | 1414 1415 | CB CG | TYR A | | | 168.157 166.933 | 0.868 | | 16.79 | A | |
| ATOM | 1415 | | TYR A | | | 166.449 | 1.561 | | 19.00 | A | |
| ATOM | 1417 | CE1 | | | | 165.265 | 2.307 | | 18.70 | A | |
| ATOM | 1418 | | TYR A | | | 166.216 | 0.947 | | 16.93 | A | |
| ATOM | 1419 | CE2 | TYR A | 295 | 192.792 | 165.035 | 1.682 | 1.00 | 21.69 | A | |
| ATOM | 1420 | CZ | TYR A | 295 | 193.916 | 164.559 | 2.357 | | 22.19 | A | |
| ATOM | 1421 | OH | TYR A | | | 163.362 | 3.046 | | 26.24 | A | |
| MOTA | 1422 | С | TYR A | | | 168.963 | -2.336 | | 10.66 | A | |
| ATOM | 1423 | 0 | TYR A | | | 168.955 | -2.741 | | 11.85 | A | |
| ATOM | 1424 | N | LEU A | | | 169.797 | -2.805 -3.807 | | 10.92 13.78 | A | |
| ATOM | 1425 1426 | CA CB | LEU A | | | 170.800 | -4.144 | | 11.44 | A A | |
| ATOM ATOM | 1427 | CG | LEU A | | | 172.488 | -2.995 | | 15.78 | A | |
| ATOM | 1428 | | LEU A | | | 173.081 | -3.411 | | 13.74 | A | |
| ATOM | 1429 | | LEU A | | | 173.585 | -2.582 | | 15.05 | A | |
| ATOM | 1430 | С | LEU A | 296 | | 170.206 | -5.108 | 1.00 | 14.17 | A | С |
| ATOM | 1431 | 0 | LEU A | | | 169.255 | -5.648 | | 12.20 | A | |
| ATOM | 1432 | N | PRO A | | | 170.783 | -5.631 | | 13.56 | A | |
| MOTA | 1433 | CD | PRO A | | | 171.841 | -5.015 | | 13.83 | A | |
| ATOM | 1434 | CA | PRO A | | | 170.302 | -6.893 -6.872 | | 12.38 14.10 | A A | |
| ATOM ATOM | 1435 1436 | CB CG | PRO A | | | 172.233 | -6.155 | | 13.16 | A | |
| MOTA | 1437 | C | PRO A | | | 170.826 | -8.083 | | 14.86 | A | |
| ATOM | 1438 | Ö | PRO A | | | 171.906 | -7.993 | | 14.20 | A | |
| ATOM | 1439 | N | PRO A | 298 | | 170.080 | -9.213 | 1.00 | 14.90 | A | N |
| MOTA | 1440 | CD | PRO A | . 298 | 193.074 | 168.838 | -9.478 | 1.00 | 13.08 | A | С |
| MOTA | 1441 | CA | PRO A | | | 170.479 | | | 12.06 | A | |
| MOTA | 1442 | CB | PRO A | | | 169.428 | | | 12.23 | A | |
| ATOM | 1443 | CG | PRO A | | | 168.254 | | | 11.96 | A | |
| MOTA | 1444 | C O | PRO A | | | 171.874 | | | 12.75 12.47 | A A | |
| ATOM ATOM | 1445 1446 | И | GLU A | | | 172.154 | | | 12.43 | A | |
| ATOM | 1447 | CA | GLU A | | | 173.447 | | | 15.93 | A | |
| ATOM | 1448 | CB | GLU A | | | 173.520 | | | 15.99 | A | |
| ATOM | 1449 | CG | GLU A | . 299 | | 3 173.211 | | 1.00 | 20.28 | A | |
| MOTA | 1450 | CD | GLU A | 299 | | 3 171.729 | | | 22.71 | A | |
| ATOM | 1451 | | . GLU A | | | 170.854 | | | 22.72 | A | |
| MOTA | 1452 | | GLU A | | | 171.450 | | | 19.63 | A | |
| ATOM | 1453 | C | GLU A | | | 174.609 | | | 17.99 | A | |
| ATOM | 1454 | 0 N | GLU A MET A | | | 7 175.706 5 174.401 | -11.147 -9.340 | | 21.24 17.80 | A A | |
| MOTA MOTA | 1455 1456 | N CA | MET A | | | 175.497 | -8.541 | | 21.17 | A A | |
| ATOM | 1456 | CB | MET A | | | 175.248 | -7.031 | | 21.87 | A | |
| ATOM | 1458 | CG | MET A | | | 175.935 | -6.417 | | 24.58 | A | _ |
| MOTA | 1459 | SD | MET A | | | 175.516 | -4.665 | | 23.96 | A | |
| ATOM | 1460 | CE | MET A | | | 175.427 | -4.097 | 1.00 | 25.92 | A | С |
| ATOM | 1461 | C | MET A | | | 175.697 | -8.845 | | 22.52 | A | |
| ATOM | 1462 | 0 | MET A | | | 176.818 | -9.034 | | 17.97 | A | |
| MOTA | 1463 | N | ILE A | 301 | 196.153 | 174.592 | -8.905 | 1.00 | 25.70 | A | N |
| | | | | | | | | | | | |

| ATOM | 1464 | CA | ILE A | | | | 174.627 | -9.160 | | 28.05 | | A | С |
|--------------|--------------|------------|------------|------------|-----|---------|------------------------|------------------|------|----------------|---|----------|--------|
| ATOM | 1465 | CB | ILE F | | | | 173.192 | -9.173 | | 31.23 | | 4 | C |
| MOTA | 1466 | | ILE F | | | | 173.228 172.525 | -9.502 -7.813 | | 33.00 34.03 | | J J | C |
| MOTA | 1467 1468 | | ILE F | | | | 172.323 | -7.813 | | 39.59 | | | č |
| ATOM ATOM | 1469 | CDI | ILE A | | | | 175.289 | | | 28.39 | | <u>-</u> | c |
| ATOM | 1470 | ō | ILE A | | | | 176.140 | | 1.00 | 28.70 | | Ą | 0 |
| ATOM | 1471 | N | GLU A | A 3 | 302 | 197.091 | 174.902 | -11.513 | | 29.15 | 2 | Ą | N |
| MOTA | 1472 | CA | GLU A | | | | 175.411 | | | 27.63 | | Ą | С |
| MOTA | 1473 | CB | GLU A | | | | 174.449 | | | 28.51 | | A | C |
| ATOM | 1474 | CG | GLU A | | | | 173.128 172.074 | | | 31.90 | | A A | C C |
| ATOM ATOM | 1475 1476 | CD OF 1 | GLU A | | | | 172.441 | | | 35.44 | | A. | õ |
| MOTA | 1477 | | GLU A | | | | 170.878 | | | 33.88 | | Ā | ō |
| ATOM | 1478 | C | GLU Z | | | | 176.817 | | 1.00 | 26.56 | 7 | A | С |
| ATOM | 1479 | 0 | GLU 2 | | | | 177.216 | | | 25.45 | | A | 0 |
| MOTA | 1480 | N | GLY I | | | | 177.553 | | | 26.68 | | A. | N |
| MOTA | 1481 | CA | GLY : | | | | 178.915 | | | 24.63 | | A. | C C |
| ATOM | 1482 | C | GLY A | | | | 179.072 180.080 | | | 26.17 25.60 | | A A | 0 |
| ATOM ATOM | 1483 1484 | N O | ARG | | | | 178.068 | | | 27.24 | | A | N |
| MOTA | 1485 | CA | ARG | | | | 178.095 | | | 26.83 | | Ą | С |
| ATOM | 1486 | CB | ARG . | | | 192.068 | 176.721 | -14.229 | 1.00 | 26.35 | | A | С |
| ATOM | 1487 | CG | ARG . | A. : | 304 | | 176.410 | | | 35.40 | | A | С |
| MOTA | 1488 | CD | ARG . | | | | 176.691 | | | 43.36 | | A. | C |
| ATOM | 1489 | NE | ARG | | | | 176.665 176.827 | | | 47.14 51.59 | | A A | N C |
| ATOM | 1490 1491 | CZ NH1 | ARG ARG | | | | 177.025 | | | 54.10 | | A. | N |
| MOTA MOTA | 1491 | | ARG | | | | 176.794 | | | 53.71 | _ | A. | N |
| ATOM | 1493 | C | ARG | | | | 178.429 | | 1.00 | 27.81 | | A | C |
| MOTA | 1494 | 0 | ARG | Α. | 304 | 191.684 | 178.391 | -11.326 | 1.00 | 29.71 | | A | 0 |
| ATOM | 1495 | N | MET | | | | 178.746 | | | 25.68 | | A | N |
| MOTA | 1496 | CA | MET | | | | 2 179.048 | | | 26.17 | | A. | C C |
| ATOM | 1497 | CB CG | MET MET | | | | ' 179.807 ' 181.155 | | | 30.29 35.60 | | A. A | C |
| ATOM ATOM | 1498 1499 | SD | MET | | | | 182.156 | | | 46.48 | | A | s |
| ATOM | 1500 | CE | MET | | | | 182.896 | | | 45.95 | | A | C |
| MOTA | 1501 | C | MET | Α | 305 | | 177.772 | | | 23.39 | | A | С |
| MOTA | 1502 | O | MET | | | | 176.721 | | | 23.54 | | A | 0 |
| MOTA | 1503 | N | HIS | | | | 177.852 | | | 21.16 17.32 | | A | N C |
| MOTA | 1504 1505 | CA CB | HIS HIS | | | | 3 176.655 2 176.035 | | | 15.79 | | A. A. | c |
| ATOM ATOM | 1505 | CG | HIS | | | | 176.853 | | - | 14.36 | | A. | c |
| MOTA | 1507 | | HIS | | | | 176.788 | | | 12.29 | | A | С |
| ATOM | 1508 | ND1 | HIS | A | 306 | | 177.880 | | 1.00 | 15.91 | | A | N |
| ATOM | 1509 | | HIS | | | | 5 178.411 | | | 13.45 | | A | С |
| ATOM | 1510 | | HIS | | | | 3 177.767 | | | 10.38 | | A. | N |
| ATOM ATOM | 1511 1512 | С 0 | HIS HIS | | | |) 176.913 3 178.063 | | | 18.65 15.46 | | A A | 0 |
| ATOM | 1513 | N | ASP | | | | 175.822 | | | 18.40 | | A | N |
| ATOM | 1514 | CA | ASP | | | | 7 175.824 | | | 20.30 | | A | С |
| MOTA | 1515 | CB | ASP | | | | 9 175.631 | | | 24.34 | | A | С |
| ATOM | 1516 | CG | ASP | | | | 174.374 | | | 30.83 | | A | C |
| ATOM | 1517 | | ASP | | | | 3 173.321 9 174.430 | | | 33.25 33.88 | | A A | 0 |
| MOTA MOTA | 1518 1519 | C | ASP | | | | 3 174.721 | | | 19.00 | | A | c |
| ATOM | 1520 | Ö | ASP | | | | 3 174.176 | | | 21.60 | | A | ō |
| ATOM | 1521 | N | GLU | | | 182.72 | 174.368 | -6.519 | 1.00 | 18.46 | | A | N |
| MOTA | 1522 | CA | GLU | | | | 7 173.358 | | | 17.19 | | A | С |
| ATOM | 1523 | CB | GLU | | | | 173.257 | | | 19.78 | | A n | C |
| ATOM | 1524 | CG | GLU | | | | 7 172.849 0 172.827 | | | 29.00 33.58 | | A A | C |
| MOTA MOTA | 1525 1526 | CD OE1 | GLU GLU | | | | L 173.800 | | | 38.06 | | A | Ö |
| ATOM | 1527 | | GLU | | | | 171.836 | | | 41.55 | | A | õ |
| ATOM | 1528 | C | GLU | | | 183.04 | 3 171.977 | -5.820 | 1.00 | 14.99 | | A | С |
| MOTA | 1529 | 0 | GLU | | | | 5 171.106 | | | 14.14 | | A | 0 |
| ATOM | 1530 | N | LYS | | | | 2 171.780 | | | 12.83 | | A | N |
| ATOM | 1531 | CA | LYS | | | | 7 170.488 L 170.376 | | | 16.26 18.82 | | A A | C |
| ATOM ATOM | 1532 1533 | CB CG | LYS LYS | | | | L 170.376 L 170.086 | | | 21.29 | | A A | C |
| P7 O11 | *223 | -00 | | •• | 555 | 2021.0 | ,0,000 | 2.000 | | | | | _ |

| ATOM | 1534 | CD | LYS | Δ | 309 | 182 3 | 15 | 168.769 | -9.041 | 1 00 | 29.52 | 70 | _ |
|------|------|-----|-------|------------|-----|---------|-------|---------|--------|------|-------|--------|-----|
| | 1535 | | | | | | | | | | | A | С |
| ATOM | | CE | LYS | | | | | 168.263 | -9.842 | 1.00 | 30.17 | A | С |
| ATOM | 1536 | ΝŻ | LYS | Α | 309 | 180.6 | 549 | 166.912 | -9.358 | 1.00 | 35.57 | Α | N |
| ATOM | 1537 | С | LYS | | | | | 170.202 | -6.826 | | 16.49 | | |
| | | | | | | | | | | | | A | С |
| ATOM | 1538 | 0 | LYS | | | 182.8 | 3 T P | 169.051 | -6.804 | 1.00 | 15.73 | A | 0 |
| MOTA | 1539 | N | VAL | Α | 310 | 186.0 | 25 | 171.233 | -6.291 | 1.00 | 15.44 | Α | N |
| ATOM | 1540 | CA | VAL | | | 187 1 | 110 | 171.020 | · | | | | |
| | | | | | | | | | -5.662 | | 13.90 | A | С |
| MOTA | 1541 | CB | VAL | Α | 310 | 188.0 |)51 | 172.358 | -5.281 | 1.00 | 15.52 | A. | С |
| ATOM | 1542 | CG1 | VAL | Α | 310 | 188.1 | 97 | 173.247 | -6.503 | 1.00 | 7.36 | A | С |
| ATOM | 1543 | | VAL | | | | | | | | | | |
| | | | | | | 18/.7 | 332 | 173.065 | -4.151 | 1.00 | 12.70 | Α | С |
| MOTA | 1544 | С | VAL | Α | 310 | 187.3 | 32 | 170.159 | -4.410 | 1.00 | 17.23 | A | С |
| ATOM | 1545 | 0 | VAL | Α | 310 | 188.0 | 800 | 169.357 | -4.083 | | 19.39 | | |
| ATOM | 1546 | N | ASP | | | | | | | | | A | 0 |
| | | | | | | | | 170.306 | -3.700 | | 14.90 | A | N |
| ATOM | 1547 | CA | ASP | A | 311 | 185.8 | 304 | 169.452 | -2.541 | 1.00 | 14.20 | A | С |
| ATOM | 1548 | CB | ASP | Α | 311 | 184.5 | 574 | 169.876 | -1.727 | | 16.81 | A. | С |
| ATOM | 1549 | CG | ASP | | | | | 171.192 | -0.974 | | | | |
| | | | | | | | | | | | 16.28 | A | С |
| ATOM | 1550 | ODT | ASP | А | 311 | 185.9 | 950 | 171.565 | -0.731 | 1.00 | 12.12 | A | 0 |
| MOTA | 1551 | OD2 | ASP | Α | 311 | 183.7 | 156 | 171.832 | -0.617 | 1.00 | 13.33 | A | 0 |
| MOTA | 1552 | С | ASP | | | | | 167.983 | -2.979 | | | | |
| | 1553 | | | | | | | | | | 14.98 | Α | С |
| ATOM | | 0 | ASP | | | 182.5 | 353 | 167.090 | -2.202 | 1.00 | 16.71 | A | 0 |
| MOTA | 1554 | N | LEU | Α | 312 | 185.1 | .62 | 167.723 | -4.205 | 1.00 | 13.32 | A | N |
| ATOM | 1555 | CA | LEU | А | 312 | 185.0 | 119 | 166.342 | -4.703 | | 13.83 | | |
| ATOM | 1556 | CB | | | | | | | | | | A | С |
| | | | LEU | | | | | 166.279 | -6.028 | 1.00 | 12.75 | Α | C |
| ATOM | 1557 | CG | LEU | | | 182.7 | 80 | 166.216 | -6.008 | 1.00 | 16.02 | Α | · C |
| ATOM | 1558 | CD1 | LEU | А | 312 | 182.2 | 69 | 164.959 | -5.273 | | 14.12 | A | Ċ |
| ATOM | 1559 | | LEU | | | | | | | | | | |
| | | | | | | | | 167.482 | -5.336 | 1.00 | 16.09 | Α | С |
| ATOM | 1560 | С | LEU | А | 312 | 186.3 | 199 | 165.749 | -4.951 | 1.00 | 13.94 | A | C |
| ATOM | 1561 | 0 | LEU | Α | 312 | 186.6 | 116 | 164.546 | -4.837 | | 15.77 | A | ō |
| ATOM | 1562 | N | TRP | | | | | 166.594 | | | | | |
| | | | | | | | | | -5.329 | | 15.19 | A | N |
| ATOM | 1563 | CA | TRP | A | 313 | 188.6 | 73 | 166.093 | -5.553 | 1.00 | 13.67 | A | С |
| ATOM | 1564 | CB | TRP | Α | 313 | 189.5 | 05 | 167.131 | -6.287 | 1.00 | 10.13 | A | С |
| ATOM | 1565 | CG | TRP | Δ | 313 | | | 166.889 | | | | | |
| | | | TRP | * | 212 | | | | -6.208 | 1.00 | | A | С |
| ATOM | 1566 | | | | | | | 166.296 | -7.214 | 1.00 | 11.32 | Α | С |
| ATOM | 1567 | | TRP | | | 193.1 | .09 | 166.370 | -6.750 | 1.00 | 10.99 | Α | С |
| ATOM | 1568 | CE3 | TRP | Α | 313 | | | 165.729 | -8.471 | 1.00 | | | Ċ |
| ATOM | 1569 | | TRP | | | | | | | | | Α | |
| | | CDI | IKE | A | 213 | | | 167.266 | -5.199 | 1.00 | 10.59 | A | С |
| ATOM | 1570 | | TRP | | | 193.0 | 83 | 166.960 | -5.513 | 1.00 | 9.03 | A | N |
| ATOM | 1571 | CZ2 | TRP | Α | 313 | 194.1 | 90 | 165.890 | -7.494 | 1.00 | 10.17 | A | С |
| ATOM | 1572 | CZ3 | TRP | А | 313 | 192.5 | 98 | 165.254 | -9.214 | | 13.43 | | |
| ATOM | 1573 | | TRP | | | | | | | | | A | C |
| | | | | | | | | 165.344 | -8.723 | | 12.05 | Α | C |
| ATOM | 1574 | С | TRP | | | | | 165.776 | -4.183 | 1.00 | 12.20 | Α | С |
| ATOM | 1575 | 0 | TRP | A | 313 | 189.8 | 03 | 164.704 | -3.983 | 1.00 | 11.38 | Α | 0 |
| ATOM | 1576 | N | SER | Α | 314 | 189.1 | 11 | 166.700 | -3.236 | | 13.68 | A | |
| ATOM | 1577 | CA | SER | | | | | 166.492 | | | | | N |
| | | | | | | | | | -1.893 | | 16.07 | A | С |
| ATOM | 1578 | CB | SER | | | 189.2 | 29 | 167.643 | -0.984 | 1.00 | 17.53 | A | C |
| ATOM | 1579 | OG | SER | Α | 314 | 190.2 | 61 | 168.612 | -0.972 | 1.00 | 25.41 | A | 0 |
| ATOM | 1580 | С | SER | | | | | 165.168 | | | | | |
| ATOM | 1581 | | | | | 100.1 | 40 | 100.100 | | | 16.32 | A | С |
| | | 0 | SER | | | | | 164.475 | -0.628 | | 15.29 | Α | 0 |
| ATOM | 1582 | N | LEU | Α | 315 | 187.9 | 07 | 164.838 | -1.517 | 1.00 | 15.55 | Α | N |
| MOTA | 1583 | CA | LEU | Α | 315 | 187.3 | 11 | 163.618 | -1.029 | | 15.03 | A | C |
| ATOM | 1584 | CB | LEU | | | | | 163.597 | | | | | |
| | | | | | | | | | -1.392 | | 15.51 | A | С |
| ATOM | 1585 | CG | LEU . | | | 184.9 | 51 | 162.599 | -0.624 | 1.00 | 17.84 | A | С |
| ATOM | 1586 | CD1 | LEU | A | 315 | 184.8 | 77 | 163.015 | 0.840 | | 17.24 | A | Č |
| ATOM | 1587 | | LEU . | | | | | 162.551 | -1.222 | | | | |
| | | | | | | | | | | | 15.53 | A | C |
| ATOM | 1588 | С | LEU . | | | 188.0 | 31 | 162.402 | -1.626 | 1.00 | 15.76 | Α | C |
| ATOM | 1589 | 0 | LEU . | Α. | 315 | 188.2 | 37 | 161.399 | -0.935 | 1.00 | 16.26 | A | 0 |
| ATOM | 1590 | N | GLY . | Δ : | 316 | 188 4 | 14 | 162.480 | -2.899 | | 13.03 | | |
| | 1591 | | | | | | | | | | | A | N |
| ATOM | | CA | GLY . | | | | | 161.357 | -3.507 | | 12.73 | A | С |
| ATOM | 1592 | C | GLY . | A : | 316 | 190.4 | 86 | 161.200 | -2.878 | 1.00 | 13.41 | A | С |
| ATOM | 1593 | 0 | GLY : | A : | 316 | 190.9 | 33 | 160.092 | -2.576 | | 11.78 | A | ō |
| ATOM | 1594 | N | VAL . | | | | | 162.329 | | | | | |
| | | | | | | | | | -2.702 | | 12.49 | A | N |
| ATOM | 1595 | | VAL A | | | | | 162.351 | -2.089 | 1.00 | 11.35 | A | С |
| MOTA | 1596 | CB | VAL 2 | Α : | 317 | 193.0 | 34 | 163.812 | -1.984 | | 11.65 | A | Ċ |
| MOTA | 1597 | | VAL A | | | | | 163.859 | -1.079 | | 10.54 | | |
| | | | | | | | | | | | | A | С |
| ATOM | 1598 | | VAL A | | | | | 164.323 | -3.360 | | 8.84 | A | С |
| ATOM | 1599 | C | VAL 2 | Α. | 317 | 192.3 | 62 | 161.759 | -0.680 | 1.00 | 12.97 | A | С |
| ATOM | 1600 | | VAL A | | | | | 160.887 | -0.280 | | 11.80 | | |
| ATOM | 1601 | | | | | | | | | | | A - | 0 |
| | | | LEU A | | | | | 162.229 | 0.052 | | 10.99 | A | N |
| ATOM | 1602 | CA | LEU A | Α : | 318 | 191.0 | 97 | 161.785 | 1.408 | 1.00 | 12.40 | A. | С |
| ATOM | 1603 | CB | LEU A | A : | 318 | 189.9 | 58 | 162.618 | 2.007 | | 15.26 | A | Č |
| | | | | | - | . = • • | | | | | | • • | ~ |
| | | | | | | | | | | | | | |

| ATOM | 1604 | CG | LEU A | 318 | 189.652 | 162.340 | 3.475 | 1.00 1 | 5.97 | A | С |
|--------------|--------------|---------|-------|-----|--------------------|--------------------|------------------|--------|-------|--------|--------|
| MOTA | 1605 | CD1 | LEU A | 318 | 190.731 | 162.990 | 4.377 | 1.00 1 | .4.54 | Α | С |
| ATOM | 1606 | CD2 | LEU A | 318 | 188.310 | 162.873 | 3.783 | 1.00 1 | 13.89 | A | С |
| ATOM | 1607 | С | LEU A | 318 | 190.760 | | 1.527 | 1.00 1 | .2.64 | A | С |
| ATOM | 1608 | 0 | LEU A | 318 | 191.232 | | 2.437 | 1.00 1 | 10.92 | A | 0 |
| MOTA | 1609 | N | CYS A | | 189.936 | | 0.617 | 1.00 1 | L2.91 | A | N |
| MOTA | 1610 | CA | CYS A | 319 | 189.547 | 158.372 | 0.623 | 1.00 1 | 15.63 | A | С |
| ATOM | 1611 | CB | CYS A | | 188.512 | | -0.479 | 1.00 2 | | A | С |
| MOTA | 1612 | SG | CYS A | | 187.933 | | -0.531 | 1.00 2 | | A | S |
| MOTA | 1613 | С | CYS A | | 190.757 | | 0.394 | 1.00 1 | | A | C |
| ATOM | 1614 | 0 | CYS A | - | 190.906 | | 1.025 | 1.00 | | A | 0 |
| ATOM | 1615 | N | TYR A | | 191.614 | | -0.527 | 1.00 | | A | N |
| ATOM | 1616 | CA | TYR A | | 192.833 | | -0.827 | 1.00 | | A | C |
| MOTA | 1617 | CB | TYR A | | 193.560 | | -1.999 | 1.00 | | A | C |
| ATOM | 1618 | CG | TYR A | | 194.879 | | -2.378 | 1.00 | | A | C C |
| ATOM | 1619 | CD1 | TYR A | | 196.014 197.213 | | -1.594 -1.906 | 1.00 | | A A | Ċ |
| ATOM | 1620 | CE1 | TYR A | | 194.978 | | -3.495 | 1.00 | | A | C |
| MOTA | 1621 1622 | CE2 | TYR A | | 196.167 | | -3.822 | 1.00 | | A | c |
| MOTA | 1623 | CZ | TYR A | | 197.287 | | -3.023 | 1.00 | | A | č |
| ATOM | 1624 | OH | TYR A | | 198.459 | | -3.325 | 1.00 | | A | ő |
| ATOM ATOM | 1625 | C | TYR A | | 193.727 | | 0.428 | 1.00 | | A | č |
| ATOM | 1626 | Õ | TYR A | | 194.217 | | 0.797 | 1.00 | | A | ō |
| ATOM | 1627 | N | GLU A | | 193.922 | | 1.083 | 1.00 | | A | N |
| MOTA | 1628 | CA | GLU A | | | 158.359 | 2.289 | 1.00 | | A | С |
| ATOM | 1629 | CB | GLU A | | | 159.798 | 2.815 | 1.00 | | A | С |
| ATOM | 1630 | CG | GLU A | | 196.109 | 160.011 | 3.685 | 1.00 | 22.02 | A | С |
| ATOM | 1631 | CD | GLU A | 321 | 196.204 | 161.394 | 4.326 | 1.00 | 27.52 | A | С |
| MOTA | 1632 | OE1 | GLU A | 321 | 195.889 | 162.413 | 3.676 | 1.00 | 30.94 | A | 0 |
| ATOM | 1633 | OE2 | GLU A | 321 | 196.621 | 161.470 | 5.494 | 1.00 | 31.35 | A | 0 |
| ATOM | 1634 | C | GLU A | 321 | | 157.470 | 3.416 | 1.00 | | A | С |
| MOTA | 1635 | 0 | GLU A | | | 156.877 | 4.166 | 1.00 | | A | 0 |
| MOTA | 1636 | N | PHE A | | | 157.384 | 3.536 | 1.00 | | A | N |
| ATOM | 1637 | CA | PHE A | | | 156.568 | 4.576 | 1.00 | | A | C |
| MOTA | 1638 | CB | PHE A | | | 156.710 | 4.570 | 1.00 | 6.70 | A | C |
| MOTA | 1639 | CG | PHE A | | | 157.975 | 5.176 | 1.00 | 6.79 | A | C |
| ATOM | 1640 | | PHE A | | | 158.836 | 5.838 | 1.00 | 7.89 | A | C |
| ATOM | 1641 | | PHE A | | | 158.312 | 5.106 | 1.00 | 8.09 | A | C |
| ATOM | 1642 | | PHE A | | | 160.011 159.497 | 6.416 5.689 | 1.00 | 6.90 | A A | c c |
| MOTA | 1643 1644 | CEZ | PHE A | | | 160.340 | 6.345 | 1.00 | 8.24 | A | c |
| ATOM ATOM | 1645 | C | PHE A | | | 155.107 | 4.398 | 1.00 | | Ā | c |
| ATOM | 1646 | Ö | PHE A | | | 154.401 | 5.375 | 1.00 | | A | ŏ |
| ATOM | 1647 | N | LEU A | | | 154.663 | 3.147 | 1.00 | | A | Ŋ |
| ATOM | 1648 | CA | LEU A | | | 153.269 | 2.830 | 1.00 | | A | С |
| ATOM | 1649 | СВ | LEU A | | | 152.923 | 1.510 | 1.00 | | А | С |
| MOTA | 1650 | CG | LEU A | 323 | 190.650 | 152.911 | 1.467 | 1.00 | 11.82 | A | С |
| ATOM | 1651 | | LEU A | | 190.149 | 152.693 | 0.033 | 1.00 | 1.00 | Α | С |
| ATOM | 1652 | | LEU A | | 190.158 | 151.799 | 2.429 | 1.00 | 8.83 | A | С |
| ATOM | 1653 | С | LEU A | | | 152.888 | 2.725 | 1.00 | | A | С |
| MOTA | 1654 | 0 | LEU A | | | 151.769 | 3.072 | 1.00 | | A | 0 |
| MOTA | 1655 | N | VAL A | | | 153.832 | 2.253 | 1.00 | | A | N |
| MOTA | 1656 | CA | VAL A | | | 153.589 | 2.028 | 1.00 | | A | C |
| MOTA | 1657 | CB | VAL A | | | 154.241 | 0.703 | 1.00 | | A | C |
| ATOM | 1658 | | VAL A | | | 153.909 | 0.365 | 1.00 | | A | C |
| ATOM | 1659 | | VAL A | | | 153.788 | -0.384 | 1.00 | | A | C |
| MOTA | 1660 | C | VAL A | | | 154.085 | 3.153 | 1.00 | | A | C |
| MOTA | 1661 | 0 | VAL A | | | 153.525 | 3.419 3.819 | 1.00 | | A | O N |
| MOTA | 1662 1663 | N | GLY A | | | 155.146 155.647 | 4.902 | 1.00 | | A A | И С |
| ATOM | 1664 | CA C | GLY A | | | 156.819 | 4.459 | 1.00 | | A | c |
| MOTA MOTA | 1665 | 0 | GLY A | | | 157.330 | 5.245 | 1.00 | | A | 0 |
| ATOM | 1666 | N | LYS A | | | 157.238 | 3.204 | 1.00 | | A | и |
| ATOM | 1667 | CA | LYS A | | | 158.399 | 2.743 | 1.00 | | A | Č |
| ATOM | 1668 | CB | LYS A | | | 158.057 | 2.468 | 1.00 | | A | Č |
| MOTA | 1669 | CG | LYS A | | | 157.016 | 1.405 | 1.00 | | A | č |
| ATOM | 1670 | CD | LYS A | | | 156.728 | 1.181 | 1.00 | | A | č |
| ATOM | 1671 | CE | LYS A | | | 155.634 | 0.108 | 1.00 | | A | Č |
| ATOM | 1672 | NZ | LYS A | | | 155.235 | -0.146 | 1.00 | | A | N |
| ATOM | 1673 | C | LYS A | | | 158.927 | 1.496 | 1.00 | | A | С |
| | | | | | | | | | | | |

| ATOM | 1674 | 0 | LYS | Α | 326 | 198.050 | 158.173 | 0.745 | 1.00 18.75 | | 7\ | ٥ |
|------|------|-----|-----|---|-----|---------|-----------|--------|--------------------------|---|----|--------|
| ATOM | 1675 | N | | | 327 | | 7 160.254 | 1.290 | 1.00 19.06 | | A | |
| ATOM | 1676 | CD | | | 327 | | 161.265 | 2.050 | 1.00 18.18 | | A. | C N |
| ATOM | 1677 | CA | | | 327 | | 160.877 | 0.111 | 1.00 16.77 | | A | c |
| ATOM | 1678 | CB | | | 327 | | 162.358 | | | | A | |
| ATOM | 1679 | CG | | | 327 | | 2 162.318 | 0.331 | 1.00 18.27 | | A | C |
| ATOM | 1680 | C | | | 327 | | 160.334 | 0.997 | 1.00 17.79 | | A | C |
| ATOM | 1681 | 0 | | | 327 | | 160.334 | -1.156 | 1.00 15.47 | | A | C |
| ATOM | 1682 | N | | | | | | -1.165 | 1.00 17.98 | | A | 0 |
| ATOM | 1683 | | | | 328 | | 160.221 | -2.256 | 1.00 15.81 | | А | N |
| | | CD | | | 328 | | 160.830 | -2.419 | 1.00 13.52 | | A | С |
| ATOM | 1684 | CA | | | 328 | | 159.699 | -3.540 | 1.00 13.75 | | A | С |
| ATOM | 1685 | CB | | | 328 | | 159.511 | -4.345 | 1.00 15.58 | | Α | С |
| MOTA | 1686 | CG | | | 328 | | 160.712 | -3.922 | 1.00 15.99 | | Α | C |
| MOTA | 1687 | C | | | 328 | | 160.502 | -4.312 | 1.00 14.29 | | A | С |
| MOTA | 1688 | 0 | | | 328 | | 5 159.947 | -5.150 | 1.00 15.51 | | Α | 0 |
| ATOM | 1689 | N | | | 329 | | 161.798 | -4.039 | 1.00 15.34 | | Α | N |
| ATOM | 1690 | CA | | | 329 | | 162.627 | -4.758 | 1.00 16.02 | | Α | С |
| ATOM | 1691 | CB | | | 329 | | 163.832 | -5.357 | 1.00 11.57 | | Α | С |
| ATOM | 1692 | CG | | | 329 | | 163.456 | -6.171 | 1.00 10.41 | | A | C |
| MOTA | 1693 | | PHE | | | | 162.822 | -7.393 | 1.00 7.22 | | Α | С |
| ATOM | 1694 | | PHE | | | 197.389 | 163.646 | -5.672 | 1.00 10.88 | | Α | С |
| ATOM | 1695 | | PHE | | | | 162.365 | -8.117 | 1.00 11.91 | | Α | С |
| ATOM | 1696 | CE2 | PHE | Α | 329 | | 163.194 | -6.387 | 1.00 9.29 | | A | С |
| MOTA | 1697 | CZ | PHE | A | 329 | | 162.548 | -7.611 | 1.00 11.49 | | Α | С |
| MOTA | 1698 | С | PHE | A | 329 | 201.774 | 163.073 | -3.896 | 1.00 18.50 | | Α | C |
| MOTA | 1699 | 0 | PHE | Α | 329 | 202.501 | . 163.999 | -4.242 | 1.00 17.82 | | A | Ō |
| MOTA | 1700 | N | GLU | Α | 330 | 201.968 | 162.411 | -2.765 | 1.00 20.96 | | A | N |
| ATOM | 1701 | CA | GLU | Α | 330 | 203.061 | 162.781 | -1.872 | 1.00 25.68 | | A | C |
| MOTA | 1702 | CB | GLU | Α | 330 | 203.042 | 161.868 | -0.653 | 1.00 28.63 | | A | Č |
| MOTA | 1703 | CG | GLU | Α | 330 | 203.889 | 162.292 | 0.527 | 1.00 35.48 | | A | č |
| MOTA | 1704 | CD | GLU | Α | 330 | 203.618 | 161.381 | 1.725 | 1.00 40.14 | | A | č |
| ATOM | 1705 | OE1 | GLU | Α | 330 | | 161.798 | 2.890 | 1.00 43.93 | | A | ő |
| MOTA | 1706 | OE2 | GLU | Α | 330 | | 160.230 | 1.490 | 1.00 43.19 | | A | ŏ |
| MOTA | 1707 | С | | | 330 | | 162.666 | -2.593 | 1.00 25.36 | | A | c |
| MOTA | 1708 | 0 | GLU | Α | 330 | | 161.627 | -3.177 | 1.00 25.32 | | A | 0 |
| ATOM | 1709 | N | | | 331 | | 163.733 | -2.551 | 1.00 23.31 | | A | N |
| MOTA | 1710 | CA | ALA | | | | 163.745 | -3.184 | 1.00 23.23 | | A | C |
| MOTA | 1711 | CB | ALA | | | | 164.479 | -4.500 | 1.00 19.73 | | A | |
| ATOM | 1712 | С | ALA | | | | 164.429 | -2.239 | 1.00 24.76 | | A | C |
| ATOM | 1713 | 0 | ALA | | | | 165.040 | -1.249 | 1.00 24.70 | • | | С |
| ATOM | 1714 | N | ASN | | | | 164.320 | -2.542 | 1.00 27.89 | | A. | 0 |
| ATOM | 1715 | CA | ASN | | | | 164.922 | -1.692 | 1.00 27.89 | | A | И |
| ATOM | 1716 | CB | ASN | | | | 164.246 | -1.975 | | | A | С |
| ATOM | 1717 | CG | ASN | | | | 162.794 | -1.504 | 1.00 32.87 1.00 37.45 | | A | C |
| ATOM | 1718 | | ASN | | | | 162.504 | -0.401 | 1.00 37.43 | | A | C |
| ATOM | 1719 | | ASN | | | | 161.883 | -2.321 | | | A | 0 |
| ATOM | 1720 | | | | | | 166.462 | -1.771 | 1.00 37.38 | | A | N |
| ATOM | 1721 | ō | ASN | | | | 167.073 | -0.928 | 1.00 29.91 1.00 29.72 | | A | C |
| ATOM | 1722 | N | THR | | | | 167.092 | -2.754 | _ | | A | 0 |
| ATOM | 1723 | CA | THR | | | | 168.544 | -2.734 | 1.00 27.34 | | A | N |
| ATOM | 1724 | CB | THR | | | | 168.968 | | 1.00 25.63 | | A | C |
| ATOM | 1725 | | THR | | | | 168.766 | -3.919 | 1.00 27.29 | | A | С |
| ATOM | 1726 | | THR | | | | 168.122 | -5.232 | 1.00 25.31 | | A | 0 |
| ATOM | 1727 | C | THR | | | | 169.099 | -3.769 | 1.00 28.40 | | A | С |
| ATOM | 1728 | 0 | THR | | | | | -3.341 | 1.00 24.25 | | A | С |
| ATOM | 1729 | N | TYR | | | | 168.355 | -3.832 | 1.00 24.65 | | A | 0 |
| ATOM | 1730 | | | | | | 170.406 | -3.177 | 1.00 22.97 | | A | N |
| ATOM | | CA | TYR | | | | 171.081 | -3.584 | 1.00 24.27 | | A | С |
| | 1731 | CB | TYR | | | | 172.557 | -3.243 | 1.00 26.40 | | A | С |
| MOTA | 1732 | CG | TYR | | | | 172.899 | -1.885 | 1.00 28.73 | | A | С |
| MOTA | 1733 | | TYR | | | | 172.639 | -0.725 | 1.00 29.53 | | Ą | С |
| ATOM | 1734 | | TYR | | | | 172.945 | 0.537 | 1.00 32.11 | | A | C |
| ATOM | 1735 | | TYR | | | | 173.476 | -1.759 | 1.00 28.50 | | 4 | С |
| ATOM | 1736 | | TYR | | | | 173.794 | -0.497 | 1.00 29.43 | | Ą | С |
| ATOM | 1737 | CZ | TYR | | | | 173.518 | 0.645 | 1.00 31.88 | | A | С |
| MOTA | 1738 | ОН | TYR | | | | 173.783 | 1.910 | 1.00 34.80 | 1 | Ą | Ō |
| MOTA | 1739 | С | TYR | | | | 170.979 | -5.088 | 1.00 25.01 | | Ā | Ċ |
| MOTA | 1740 | 0 | TYR | | | | 170.712 | -5.567 | 1.00 24.09 | | A. | ō |
| ATOM | 1741 | N | GLN | | | | 171.221 | -5.831 | 1.00 24.15 | | Ā | N |
| MOTA | 1742 | CA | GLN | | | | 171.183 | -7.272 | 1.00 26.26 | | Ą | Ċ |
| ATOM | 1743 | CB | GLN | Α | 335 | 208.763 | 171.616 | -7.820 | 1.00 30.16 | | 4 | Č |
| | | | | | | | | | | | | - |

| MOTA | 1744 | CG | GLN A | A | 335 | 208.69 | 0 | 172.407 | -9.123 | 1.00 | 37.20 | | A | С |
|------|--------------|-----|-------|----|-----|--------|-----|---------|---------|------|-------|---|----|---|
| ATOM | 1745 | | GLN A | | | 209.93 | 8 | 173.249 | -9.353 | 1.00 | 44.29 | | A | С |
| ATOM | 1746 | | GLN I | | | | | 172.716 | -9.361 | 1.00 | 45.86 | | Α | 0 |
| | 1747 | | GLN A | | | | | 174.581 | -9.540 | | 45.65 | | A | N |
| MOTA | | | | | | | | 169.785 | -7.766 | | 24.06 | | A | C |
| MOTA | 1748 | C | GLN A | | | | | | | | 20.60 | | Α | ō |
| MOTA | 1749 | 0 | GLN | | | | | 169.643 | -8.661 | | | | | |
| ATOM | 1750 | N | GLU | | | | | 168.746 | -7.179 | | 23.21 | | Α | И |
| ATOM | 1751 | CA | GLU | A | 336 | | | 167.407 | -7.624 | | 22.61 | | Α | С |
| MOTA | 1752 | CB | GLU : | A | 336 | 208.18 | 3 | 166.360 | -7.022 | | 19.74 | | Α | С |
| MOTA | 1753 | CG | GLU : | Α | 336 | | | 164.932 | -7.350 | 1.00 | 27.97 | | A | С |
| ATOM | 1754 | CD | GLU . | A. | 336 | 207.85 | 2 | 164.603 | -8.845 | 1.00 | 35.28 | | Α | С |
| ATOM | 1755 | OEL | GLU . | A | 336 | 207.23 | 1 | 163.579 | -9.236 | 1.00 | 38.15 | | A | 0 |
| ATOM | 1756 | | GLU | | | 208.50 | 8 | 165.350 | -9.628 | 1.00 | 39.74 | | Α | 0 |
| MOTA | 1757 | C | GLU | | | | | 167.056 | -7.327 | 1.00 | 23.14 | | Α | С |
| ATOM | 1758 | Õ | GLU | | | | | 166.363 | -8.124 | | 23.03 | | Α | 0 |
| | 1759 | Ŋ | THR | | | | | 167.517 | -6.196 | | 21.09 | | A | N |
| ATOM | | | | | | | | 167.229 | -5.868 | | 21.21 | | A | C |
| ATOM | 1760 | CA | THR | | | | | | -4.380 | | 22.66 | | A | č |
| MOTA | 1761 | CB | THR | | | | | 167.589 | | | | | | Ö |
| ATOM | 1762 | | THR | | | | | 166.744 | -3.537 | | 24.71 | | A | |
| ATOM | 1763 | CG2 | THR | | | | | 167.366 | -4.030 | | 16.15 | | A | C |
| MOTA | 1764 | С | THR | A | 337 | | | 167.944 | -6.855 | | 19.71 | | A | C |
| ATOM | 1765 | 0 | THR | Α | 337 | | | 167.329 | -7.346 | | 21.88 | | A | 0 |
| ATOM | 1766 | N | TYR | Α | 338 | | | 169.210 | -7.171 | 1.00 | 17.76 | | A | N |
| ATOM | 1767 | CA | TYR | Α | 338 | 202.40 |) 4 | 169.982 | -8.151 | 1.00 | 17.94 | | Α | C |
| MOTA | 1768 | CB | TYR | A | 338 | 203.05 | 51 | 171.348 | -8.416 | 1.00 | 19.72 | | Α | С |
| ATOM | 1769 | CG | TYR | A | 338 | 202.92 | 24 | 172.309 | -7.282 | 1.00 | 21.47 | | A | С |
| ATOM | 1770 | | TYR | | | 203.92 | 27 | 173.231 | -7.014 | 1.00 | 26.12 | | A | С |
| ATOM | 1771 | CE1 | | | | 203.78 | 30 | 174.172 | -6.003 | 1.00 | 31.99 | | Α | С |
| MOTA | 1772 | - | TYR | | | | | 172.333 | -6.506 | | 23.72 | | Α | С |
| | 1773 | | TYR | | | | | 173.256 | -5.498 | | 28.25 | | A | C |
| ATOM | | CZ | | | 338 | | | 174.184 | -5.255 | | 32.26 | | A | Č |
| MOTA | 1774 | | | | | | | 175.197 | -4.343 | | 37.49 | | A | ŏ |
| MOTA | 1775 | OH | | | 338 | | | | | | 17.24 | | A | Ċ |
| MOTA | 1776 | C | | | 338 | | | 169.248 | -9.480 | | | | | |
| ATOM | 1777 | 0 | | | 338 | | | 169.202 | | | 17.93 | | A | 0 |
| MOTA | 1778 | N | | | 339 | | | 168.704 | -9.869 | | 18.06 | | A | N |
| MOTA | 1779 | CA | LYS | Α | 339 | | | 167.967 | | | 15.13 | | A | C |
| MOTA | 1780 | CB | LYS | Α | 339 | | | 167.521 | | | 15.66 | | A | С |
| MOTA | 1781 | CG | LYS | Α | 339 | 205.2 | 32 | 166.761 | -12.647 | 1.00 | 25.11 | | Ą | С |
| MOTA | 1782 | CD | LYS | Α | 339 | 206.6 | 75 | 166.164 | -12.838 | 1.00 | 28.61 | | A | С |
| MOTA | 1783 | CE | LYS | Α | 339 | 207.7 | 36 | 167.232 | -12.973 | 1.00 | 30.48 | | A | С |
| ATOM | 1784 | NZ | LYS | Α | 339 | 209.0 | 81 | 166.590 | -13.128 | 1.00 | 37.06 | | A | N |
| ATOM | 1785 | C | LYS | Α | 339 | 202.7 | 34 | 166.747 | -11.110 | 1.00 | 15.66 | | A | С |
| ATOM | 1786 | 0 | LYS | Α | 339 | 201.9 | 99 | 166.520 | -12.062 | 1.00 | 16.79 | | A | 0 |
| ATOM | 1787 | И | | | 340 | | | 165.963 | | 1.00 | 14.01 | | A | N |
| ATOM | 1788 | CA | | | 340 | | | 164.754 | -9.941 | | 17.25 | | A | C |
| ATOM | 1789 | CB | | | 340 | | | 163.917 | -8.749 | | 17.92 | | A | C |
| | | | | | 340 | | | 163.112 | | | 20.94 | Y | A | č |
| ATOM | 1790 1791 | CG | | | 340 | | | 162.632 | -7.805 | | 26.11 | | A | Ċ |
| MOTA | | | | | | | | 162.024 | | | 30.74 | | A | N |
| ATOM | 1792 | NE | | | 340 | | | | -7.014 | | 34.14 | | A | C |
| ATOM | 1793 | CZ | | | 340 | | | 161.430 | -5.805 | | 36.45 | | A | N |
| MOTA | 1794 | | ARG | | | | | 161.387 | | | | | | |
| ATOM | 1795 | | ARG | | | | | 160.886 | -7.219 | | 32.82 | | A | N |
| ATOM | 1796 | C | | | 340 | | | 164.980 | -9.876 | | 16.32 | | A | С |
| MOTA | 1797 | 0 | | | 340 | | | 164.177 | | | 13.54 | | A | 0 |
| MOTA | 1798 | N | ILE | Α | 341 | | | 166.068 | -9.242 | | 16.44 | | A | N |
| MOTA | 1799 | CA | ILE | Α | 341 | | | 166.396 | | | 15.90 | | A | С |
| ATOM | 1800 | CB | ILE | Α | 341 | 198.4 | 25 | 167.544 | -8.133 | 1.00 | 14.61 | | Α | С |
| MOTA | 1801 | CG2 | ILE | Α | 341 | 197.0 | 31 | 168.173 | -8.284 | 1.00 | 10.21 | | Α | C |
| ATOM | 1802 | | ILE | | | | | 166.991 | | 1.00 | 9.86 | | A | С |
| ATOM | 1803 | | ILE | | | | | 168.066 | | | 10.30 | | Α | C |
| ATOM | 1804 | C | | | 341 | | | 166.813 | | | 16.94 | | A | Ċ |
| MOTA | 1805 | ő | | | 341 | | | 166.346 | | | 15.49 | | A | ō |
| | 1806 | N | | | 342 | | | 167.677 | | | 17.49 | | A | N |
| MOTA | | | | | 342 | | | 168.185 | | | 19.50 | | A | Ċ |
| MOTA | 1807 | CA | | | | | | 169.153 | | | 19.12 | | A | C |
| ATOM | 1808 | CB | | | 342 | | | | | | 28.84 | | | |
| MOTA | 1809 | OG | | | 342 | | | 169.899 | | | | | A. | 0 |
| ATOM | 1810 | C | | | 342 | | | 167.065 | | | 18.65 | | A | C |
| MOTA | 1811 | 0 | | | 342 | | | 167.157 | | | 17.15 | | A | 0 |
| MOTA | 1812 | N | | | 343 | | | 166.027 | | | 16.76 | | A | N |
| MOTA | 1813 | CA | ARG | A | 343 | 199.1 | 87 | 164.881 | -14.291 | Ι.00 | 16.82 | | A | С |

| ATOM | 1814 | СВ | ARG A | 343 | 200.563 | 164.214 | -14.356 | 1.00 | 19.40 | Α | С |
|------|------|-----|-------|-------|---------|---------|---------|------|-------|---|---|
| ATOM | 1815 | CG | ARG A | | | 165.034 | | | 20.85 | A | C |
| ATOM | 1816 | CD | ARG A | | | 164.139 | | | 22.63 | A | Ċ |
| ATOM | 1817 | NE | ARG A | | | 164.667 | | | 29.67 | A | N |
| ATOM | 1818 | CZ | ARG A | | | 163.964 | | | 29.30 | A | Ċ |
| | 1819 | | ARG A | | | 162.702 | | | 27.60 | A | N |
| MOTA | | | | | | 164.521 | | | 30.90 | A | N |
| MOTA | 1820 | | ARG A | | | | | | | | C |
| ATOM | 1821 | C | ARG A | | | 163.833 | | | 17.95 | A | |
| MOTA | 1822 | 0 | ARG A | | | 162.927 | | | 18.61 | A | 0 |
| ATOM | 1823 | N | VAL A | | | 163.963 | | | 16.47 | A | N |
| MOTA | 1824 | CA | VAL A | | | 163.027 | | | 15.15 | A | C |
| ATOM | 1825 | CB | VAL A | | | 162.882 | | | 14.04 | A | С |
| MOTA | 1826 | | VAL A | | | 161.919 | | | 14.73 | A | С |
| ATOM | 1827 | | VAL A | | | 164.217 | | | 14.41 | A | C |
| ATOM | 1828 | С | VAL A | | | 161.702 | | | 19.48 | Α | С |
| ATOM | 1829 | 0 | VAL A | | | 160.697 | | | 17.59 | A | 0 |
| MOTA | 1830 | N | GLU A | | | 161.733 | | | 20.63 | A | N |
| MOTA | 1831 | CA | GLU A | 345 | | 160.600 | | 1.00 | 21.68 | Α | С |
| MOTA | 1832 | CB | GLU A | | | 161.116 | | | 22.57 | A | С |
| MOTA | 1833 | CG | GLU A | | | 160.066 | | 1.00 | 29.02 | A | С |
| MOTA | 1834 | CD | GLU A | 345 | 203.609 | 160.693 | -12.596 | 1.00 | 34.43 | A | С |
| MOTA | 1835 | | GLU A | | 203.572 | 161.826 | -13.143 | 1.00 | 41.54 | Α | 0 |
| ATOM | 1836 | OE2 | GLU A | 345 | 204.677 | 160.062 | -12.448 | 1.00 | 34.88 | A | 0 |
| MOTA | 1837 | С | GLU A | 345 | 199.906 | 159.839 | -9.990 | 1.00 | 21.02 | A | С |
| MOTA | 1838 | 0 | GLU A | 345 | 200.516 | 160.289 | -9.009 | 1.00 | 22.86 | Α | 0 |
| MOTA | 1839 | N | PHE A | 346 | 199.260 | 158.679 | -9.953 | 1.00 | 20.71 | A | N |
| MOTA | 1840 | CA | PHE A | 346 | 199.268 | 157.868 | -8.730 | 1.00 | 20.54 | Α | С |
| ATOM | 1841 | CB | PHE A | 346 | 198.272 | 158.454 | -7.705 | 1.00 | 19.53 | A | С |
| ATOM | 1842 | CG | PHE A | 346 | 196.835 | 158.138 | -8.013 | 1.00 | 21.11 | A | C |
| ATOM | 1843 | CD1 | PHE A | 346 | 196.203 | 157.064 | -7.403 | 1.00 | 22.02 | A | C |
| ATOM | 1844 | CD2 | PHE A | 346 | 196.130 | 158.888 | -8.936 | 1.00 | 18.36 | A | С |
| ATOM | 1845 | CE1 | PHE A | 346 | 194.878 | 156.744 | -7.713 | 1.00 | 24.10 | A | С |
| ATOM | 1846 | CE2 | PHE A | 346 | 194.807 | 158.574 | -9.253 | 1.00 | 23.07 | Α | C |
| MOTA | 1847 | CZ | PHE A | 346 | 194.181 | 157.500 | -8.640 | 1.00 | 22.64 | A | С |
| ATOM | 1848 | С | PHE A | 346 | 198.893 | 156.424 | -9.065 | 1.00 | 19.41 | A | C |
| ATOM | 1849 | 0 | PHE A | 346 | 198.376 | 156.142 | -10.153 | 1.00 | 21.26 | A | 0 |
| ATOM | 1850 | N | THR A | 347 | 199.158 | 155.512 | -8.137 | 1.00 | 17.51 | A | N |
| ATOM | 1851 | CA | THR A | 347 | 198.809 | 154.113 | -8.335 | 1.00 | 15.60 | A | C |
| ATOM | 1852 | CB | THR A | 347 | 200.042 | 153.259 | -8.736 | 1.00 | 17.00 | A | С |
| ATOM | 1853 | OG1 | THR A | 347 | 201.113 | 153.494 | -7.812 | 1.00 | 20.54 | A | 0 |
| ATOM | 1854 | CG2 | THR A | 347 | 200.506 | 153.617 | -10.145 | 1.00 | 14.88 | A | С |
| ATOM | 1855 | С | THR A | 347 | 198.245 | 153.623 | -7.026 | 1.00 | 14.01 | A | С |
| ATOM | 1856 | 0 | THR A | 347 | | 154.324 | -6.030 | 1.00 | 14.17 | A | 0 |
| ATOM | 1857 | N | PHE A | 348 | | 152.434 | -7.029 | 1.00 | 14.30 | Α | N |
| ATOM | 1858 | CA | PHE A | 348 | 197.097 | 151.875 | -5.809 | 1.00 | 15.62 | Α | C |
| ATOM | 1859 | СВ | PHE A | | | 151.335 | -6.022 | | 13.71 | A | С |
| ATOM | 1860 | CG | PHE A | | | 152.345 | -6.553 | | 14.90 | A | С |
| ATOM | 1861 | | PHE A | | | 152.496 | -7.926 | | 14.48 | A | С |
| ATOM | 1862 | | PHE A | | | 153.115 | -5.678 | | 14.25 | A | С |
| ATOM | 1863 | | PHE A | | | 153.399 | -8.421 | | 13.33 | A | |
| ATOM | 1864 | | PHE A | | | 154.020 | -6.160 | | 12.61 | A | |
| ATOM | 1865 | CZ | PHE A | 348 | | 154.162 | -7.530 | | 13.12 | A | С |
| ATOM | 1866 | С | PHE A | . 348 | | 150.690 | -5.379 | 1.00 | 17.39 | A | C |
| ATOM | 1867 | 0 | PHE A | | | 149.986 | -6.222 | | 17.79 | A | 0 |
| ATOM | 1868 | N | PRO A | | | 150.478 | -4.060 | | 19.22 | Α | N |
| MOTA | 1869 | CD | PRO A | 349 | 197.716 | 151.428 | -2.984 | 1.00 | 20.64 | Α | C |
| ATOM | 1870 | CA | PRO A | 349 | | 149.326 | ~3.550 | 1.00 | 18.28 | Α | С |
| ATOM | 1871 | CB | PRO A | 349 | | 149.550 | -2.034 | 1.00 | 19.47 | Α | С |
| MOTA | 1872 | CG | PRO A | 349 | | 151.042 | -1.874 | 1.00 | 21.78 | Α | С |
| MOTA | 1873 | С | PRO A | | | 148.144 | -3.906 | 1.00 | 18.89 | A | C |
| MOTA | 1874 | 0 | PRO A | | 196.765 | 148.365 | -4.282 | 1.00 | 18.06 | Α | 0 |
| ATOM | 1875 | N | ASP A | | | 146.901 | -3.778 | | 22.60 | A | N |
| MOTA | 1876 | CA | ASP A | | | 145.780 | -4.137 | | 24.29 | A | С |
| ATOM | 1877 | CB | ASP A | | | 144.494 | -4.298 | | 28.79 | Α | С |
| MOTA | 1878 | CG | ASP A | | | 144.608 | -5.404 | | 33.91 | A | С |
| ATOM | 1879 | | ASP A | | | 143.575 | -5.741 | | 33.53 | A | 0 |
| MOTA | 1880 | | ASP A | | | 145.733 | -5.928 | | 35.29 | A | 0 |
| MOTA | 1881 | С | ASP A | | | 145.489 | -3.238 | | 23.99 | A | C |
| MOTA | 1882 | 0 | ASP A | | | 144.835 | -3.671 | | 23.48 | A | 0 |
| MOTA | 1883 | N | PHE A | 351 | 196.279 | 145.964 | -2.003 | 1.00 | 22.20 | A | N |
| | | | | | | | | | | | |

| MOTA | 1884 | CA | PHE | | | | | 145.636 | | 171 | | 23.75 | A | C |
|--------------|--------------|-----------|------------|---|------------|-----|-------|--------------------|-----|--------------|------|----------------|--------|--------|
| MOTA | 1885 | CB | PHE | | | | | 145.662 | | 300 | | 22.72 | A | C |
| MOTA | 1886 1887 | CG CD1 | PHE | | | | | 146.956 147.151 | | .738 .756 | | 17.28 | A A | C |
| ATOM ATOM | 1888 | | PHE | | | | | 147.131 | | 111 | | 19.08 | A | C |
| MOTA | 1889 | | PHE | | | | | 148.379 | | 142 | | 21.72 | A | c |
| ATOM | 1890 | | PHE | | | _ | | 149.217 | | 497 | | 19.31 | A | c |
| ATOM | 1891 | CZ | PHE | | | | | 149.417 | | 515 | | 20.15 | A | Č |
| ATOM | 1892 | C | PHE | | | | | 146.509 | | 382 | | 24.86 | A | C |
| MOTA | 1893 | 0 | PHE | | | | | 146.215 | | 820 | | 26.36 | A | 0 |
| ATOM | 1894 | N | VAL | A | 352 | 193 | .999 | 147.575 | -2. | . 174 | 1.00 | 22.98 | A | N |
| ATOM | 1895 | CA | VAL | A | 352 | 192 | 845 | 148.431 | -2. | . 428 | 1.00 | 22.53 | A | С |
| MOTA | 1896 | CB | VAL | | | | | 149.810 | | . 976 | | 19.91 | A | С |
| MOTA | 1897 | | VAL | | | | | 150.680 | | . 293 | | 15.94 | A | С |
| ATOM | 1898 | | VAL | | | | | 150.489 | | . 936 | | 17.58 | A | C |
| ATOM | 1899 | C | VAL | | | | | 147.702 | | . 416 | | 22.85 | A | C |
| ATOM | 1900 | 0 | VAL | | | | | 147.406 | | .541 | | 25.56 | A | 0 |
| ATOM ATOM | 1901 1902 | N CA | THR THR | | | | | 147.393 146.668 | | .985 .833 | | 20.20 | A A | N C |
| ATOM | 1903 | CB | THR | | | | | 146.264 | | .059 | | 18.44 | A | c |
| ATOM | 1904 | | THR | | | | | 147.445 | | .740 | | 19.14 | A | ŏ |
| ATOM | 1905 | | THR | | | | | 145.544 | | .786 | | 15.00 | A | C |
| ATOM | 1906 | С | THR | | | | | 147.452 | | .049 | | 23.02 | A | C |
| ATOM | 1907 | 0 | THR | Α | 353 | 189 | .525 | 148.665 | -5. | . 144 | 1.00 | 21.93 | A | 0 |
| MOTA | 1908 | N | GLU | A | 354 | 188 | . 685 | 146.733 | -5. | .960 | 1.00 | 23.98 | A | N |
| MOTA | 1909 | CA | GLU | | | | | 147.274 | | .208 | | 25.43 | A | С |
| MOTA | 1910 | CB | GLU | | | | | 146.130 | | .001 | | 30.21 | A | C |
| ATOM | 1911 | CG | | | 354 | | | 146.540 | | . 261 | | 37.82 | A. | C |
| ATOM | 1912 | CD | | | 354 | | | 145.351 | | .890 | | 41.79 | A. | C |
| ATOM ATOM | 1913 1914 | OE1 | GLU GLU | | | | | 145.472 144.281 | | . 224 | | 43.51 44.80 | A A | 0 |
| ATOM | 1915 | C | | | 354 | | | 148.424 | | .055 | | 24.34 | A | Ċ |
| ATOM | 1916 | ŏ | | | 354 | | | 149.386 | | .840 | | 24.85 | A | 0 |
| ATOM | 1917 | N | | | 355 | | | 148.303 | | .065 | | 20.96 | A | N |
| ATOM | 1918 | CA | | | 355 | | | 149.314 | | .842 | | 13.82 | A | C |
| MOTA | 1919 | С | GLY | A | 355 | 185 | .908 | 150.595 | -5 | .333 | 1.00 | 16.94 | A | С |
| ATOM | 1920 | 0 | GLY | A | 355 | 185 | .529 | 151.694 | -5 | .760 | 1.00 | 13.60 | A | 0 |
| ATOM | 1921 | N | ALA | Α | 356 | | | 150.473 | | . 425 | 1.00 | 15.45 | A | N |
| ATOM | 1922 | CA | | | 356 | | | 151.674 | | . 909 | | 19.10 | A | С |
| MOTA | 1923 | CB | | | 356 | | | 151.326 | | .761 | | 18.64 | A | C |
| MOTA | 1924 | C | | | 356 | | | 152.381 | | .068 | | 19.08 | A | C |
| ATOM ATOM | 1925 1926 | O N | | | 356 357 | | | 153.604 151.611 | | .951 | | 16.84 18.44 | A A | O N |
| ATOM | 1927 | CA | | | 357 | | | 152.184 | | .100 | | 18.13 | A | C |
| ATOM | 1928 | CB | | | 357 | | | 151.113 | | .881 | | 16.00 | A | Č |
| ATOM | 1929 | CG | | | 357 | | | 150.447 | | .112 | | 15.75 | A | Ċ |
| MOTA | 1930 | CD | | | 357 | | | 149.414 | | 941 | | 14.24 | A | C |
| ATOM | 1931 | NE | ARG | A | 357 | 193 | .120 | 148.721 | -7 | .139 | 1.00 | 18.00 | A | N |
| ATOM | 1932 | CZ | | | 357 | | | 148.203 | | .607 | | 18.74 | A | С |
| ATOM | 1933 | | ARG | | | | | 148.285 | | .898 | | 21.62 | A | N |
| MOTA | 1934 | | ARG | | | | | 147.622 | | .768 | | 20.49 | A | N |
| ATOM | 1935 | C | | | 357 357 | | | 152.856 153.878 | | .062 | | 17.28 16.53 | A | C |
| ATOM ATOM | 1936 1937 | O N | | | 358 | | | 152.272 | | .261 | | 17.73 | A A | Ŋ |
| ATOM | 1938 | CA | | | 358 | | | 152.887 | | .176 | | 17.93 | A | C |
| ATOM | 1939 | CB | | | 358 | | | 152.024 | | .389 | | 21.16 | A | č |
| ATOM | 1940 | CG | | | 358 | | | 152.688 | | | | 23.93 | A | Č |
| MOTA | 1941 | | ASP | | | | | 152.671 | | | 1.00 | 29.93 | A | 0 |
| ATOM | 1942 | OD2 | ASP | A | 358 | | | 153.257 | | .840 | 1.00 | 22.82 | A | 0 |
| ATOM | 1943 | С | | | 358 | | | 154.234 | | .611 | | 17.83 | A | С |
| ATOM | 1944 | 0 | | | 358 | | | 155.206 | | . 348 | | 20.18 | A | 0 |
| MOTA | 1945 | N | | | 359 | | | 154.299 | | .303 | | 16.69 | A | N |
| ATOM | 1946 | CA | | | 359 | | | 155.543 | | .680 | | 15.23 | A | С |
| ATOM | 1947 | CB | | | 359 | | | 155.292 156.568 | | .250 .482 | | 13.90 15.76 | A n | C |
| ATOM ATOM | 1948 1949 | CG CD1 | LEU | | 359 359 | | | 157.164 | | .105 | | 14.16 | A A | C |
| ATOM | 1949 | | LEU | | | | | 156.266 | | .027 | | 16.19 | A | c |
| ATOM | 1951 | C | | | 359 | | | 156.623 | | 646 | | 15.38 | A | c |
| ATOM | 1952 | Ö | | | 359 | | | 157.740 | | 071 | | 16.61 | A | ō |
| ATOM | 1953 | N | | | 360 | | | 156.300 | | .132 | | 15.08 | A | N |

| | | | | | | | | _ | |
|------|------|-----|-------------|------------|----------|---------|------------|---|---|
| MOTA | 1954 | CA | ILE A 360 | 188.737 15 | 7.280 | -6.054 | 1.00 16.09 | A | С |
| ATOM | 1955 | CB | ILE A 360 | 189.972 15 | 6.694 | -5.305 | 1.00 13.18 | A | С |
| MOTA | 1956 | | ILE A 360 | 191.132 15 | | -5.348 | 1.00 8.95 | A | С |
| | | | ILE A 360 | 189.613 15 | | -3.843 | 1.00 11.43 | A | С |
| ATOM | 1957 | | | | | | | | č |
| MOTA | 1958 | | ILE A 360 | 190.486 15 | | -3.211 | 1.00 15.13 | A | |
| ATOM | 1959 | С | ILE A 360 | 189.126 15 | 57.752 | -7.457 | 1.00 18.67 | A | С |
| MOTA | 1960 | 0 | ILE A 360 | 189.433 15 | 68.935 | -7.652 | 1.00 19.76 | A | 0 |
| ATOM | 1961 | N | SER A 361 | 189.099 15 | 56.841 | -8.427 | 1.00 17.86 | A | N |
| | | | SER A 361 | 189.437 15 | | -9.792 | 1.00 17.51 | A | С |
| MOTA | 1962 | CA | | | | | | | č |
| MOTA | 1963 | CB | SER A 361 | 189.511 15 | | | 1.00 18.17 | A | |
| MOTA | 1964 | OG | SER A 361 | 190.686 19 | 55.223 · | -10.384 | 1.00 20.30 | A | 0 |
| ATOM | 1965 | С | SER A 361 | 188.438 19 | 58.163 | -10.382 | 1.00 18.63 | A | С |
| MOTA | 1966 | 0 | SER A 361 | 188.805 19 | 59.011 | -11.209 | 1.00 19.26 | A | 0 |
| | 1967 | N | ARG A 362 | 187.175 19 | | -9.977 | 1.00 18.68 | A | N |
| MOTA | | | | 186.156 19 | | | 1.00 17.96 | A | Ċ |
| MOTA | 1968 | CA | ARG A 362 | | | | | | |
| MOTA | 1969 | CB | ARG A 362 | 184.740 15 | | | 1.00 18.15 | A | C |
| ATOM | 1970 | CG | ARG A 362 | 184.389 1 | 57.189 | -10.948 | 1.00 21.87 | A | С |
| MOTA | 1971 | CD | ARG A 362 | 182.950 1 | 56.762 | -10.710 | 1.00 24.92 | Α | С |
| ATOM | 1972 | NE | ARG A 362 | 182.669 1 | 55.532 | -11.449 | 1.00 31.73 | A | N |
| | | CZ | ARG A 362 | 182.150 1 | | | 1.00 35.25 | A | С |
| MOTA | 1973 | | | 181.805 1 | | | 1.00 34.91 | A | N |
| ATOM | 1974 | | ARG A 362 | | | | | | |
| MOTA | 1975 | NH2 | ARG A 362 | 182.052 1 | | | 1.00 35.12 | A | N |
| MOTA | 1976 | С | ARG A 362 | 186.287 1 | 60.332 | -9.817 | 1.00 16.66 | A | С |
| MOTA | 1977 | 0 | ARG A 362 | 186.086 1 | 61.367 | -10.452 | 1.00 21.59 | A | 0 |
| | 1978 | N | LEU A 363 | 186.602 1 | | -8.527 | 1.00 15.31 | A | N |
| ATOM | | | | 186.726 1 | | -7.814 | 1.00 15.39 | A | c |
| MOTA | 1979 | CA | LEU A 363 | | | | | | c |
| ATOM | 1980 | CB | LEU A 363 | 186.758 1 | | -6.295 | 1.00 13.54 | A | |
| ATOM | 1981 | CG | LEU A 363 | 185.452 1 | | -5.638 | 1.00 14.63 | A | С |
| ATOM | 1982 | CD1 | LEU A 363 | 185.723 1 | 60.358 | -4.216 | 1.00 12.73 | Α | С |
| ATOM | 1983 | CD2 | LEU A 363 | 184.423 1 | | -5.613 | 1.00 7.80 | A | С |
| | | | LEU A 363 | 187.989 1 | | -8.252 | 1.00 16.50 | A | С |
| MOTA | 1984 | C | | | | | | A | ō |
| MOTA | 1985 | 0 | LEU A 363 | 188.033 1 | | -8.252 | 1.00 16.60 | | |
| MOTA | 1986 | N | LEU A 364 | 189.008 1 | 61.597 | -8.656 | 1.00 17.23 | A | N |
| ATOM | 1987 | CA | LEU A 364 | 190.285 1 | 62.182 | -9.051 | 1.00 20.15 | A | С |
| MOTA | 1988 | СВ | LEU A 364 | 191.419 1 | 61.335 | -8.467 | 1.00 18.29 | A | C |
| ATOM | 1989 | CG | LEU A 364 | 191.504 1 | | -6.926 | 1.00 20.11 | A | С |
| | | | | 192.737 1 | | -6.509 | 1.00 16.10 | A | С |
| MOTA | 1990 | | LEU A 364 | | | | | | č |
| MOTA | 1991 | CD2 | LEU A 364 | 191.576 1 | | -6.413 | 1.00 16.30 | A | |
| MOTA | 1992 | С | LEU A 364 | 190.474 1 | 62.393 | -10.557 | 1.00 19.92 | A | С |
| ATOM | 1993 | 0 | LEU A 364 | 191.511 1 | 62.052 | -11.143 | 1.00 20.12 | Α | 0 |
| ATOM | 1994 | N | LYS A 365 | 189.450 1 | 62.967 | -11.169 | 1.00 19.36 | Α | N |
| ATOM | 1995 | CA | LYS A 365 | 189.461 1 | | | 1.00 19.00 | Α | С |
| | | | LYS A 365 | 188.039 1 | | | 1.00 22.47 | A | С |
| ATOM | 1996 | CB | | 187.417 1 | | | 1.00 23.42 | A | Ċ |
| MOTA | 1997 | CG | LYS A 365 | | | | | | |
| ATOM | 1998 | CD | LYS A 365 | 188.039 1 | | | 1.00 23.31 | A | С |
| ATOM | 1999 | CE | LYS A 365 | 187.320 1 | .59.930 | -14.693 | 1.00 24.89 | A | С |
| ATOM | 2000 | NZ | LYS A 365 | 187.970 1 | 59.249 | -15.851 | 1.00 30.35 | A | N |
| ATOM | 2001 | C | LYS A 365 | 190.039 1 | 64.670 | -12.715 | 1.00 18.75 | A | С |
| | | | LYS A 365 | 189.654 1 | | | | A | 0 |
| ATOM | 2002 | 0 | | | | | | | |
| MOTA | 2003 | N | HIS A 366 | 190.949 1 | | | 1.00 17.07 | A | N |
| ATOM | 2004 | CA | HIS A 366 | 191.568 1 | | | 1.00 17.25 | A | C |
| ATOM | 2005 | CB | HIS A 366 | 192.611 1 | .66.038 | -15.043 | 1.00 15.66 | A | С |
| ATOM | 2006 | CG | HIS A 366 | 193.302 1 | .67.331 | -15.352 | 1.00 18.71 | Α | С |
| ATOM | 2007 | | HIS A 366 | 194.437 1 | 67.877 | -14.849 | 1.00 17.17 | A | С |
| | 2008 | | HIS A 366 | 192,763 1 | | | 1.00 19.79 | A | N |
| MOTA | | | | | | | | A | Ċ |
| ATOM | 2009 | | HIS A 366 | 193.530 1 | | | | | |
| MOTA | 2010 | NE2 | 2 HIS A 366 | 194.552 1 | | | 1.00 18.20 | A | N |
| ATOM | 2011 | С | HIS A 366 | 190.493 1 | | | | A | С |
| ATOM | 2012 | 0 | HIS A 366 | 190.553 1 | .68.334 | -13.864 | 1.00 14.94 | A | 0 |
| ATOM | 2013 | N | ASN A 367 | 189.500 1 | | | 1.00 19.37 | A | N |
| | | | ASN A 367 | 188.436 1 | | | | A | c |
| ATOM | 2014 | CA | | | | | | | Č |
| ATOM | 2015 | CB | ASN A 367 | 187.841 1 | | | | A | |
| ATOM | 2016 | | ASN A 367 | 186.929 1 | | | | A | С |
| ATOM | 2017 | OD1 | L ASN A 367 | 185.990 1 | 68.718 | -16.827 | 1.00 34.30 | A | 0 |
| ATOM | 2018 | | ASN A 367 | 187.209 1 | 168.611 | -18.688 | 1.00 31.42 | A | N |
| | 2019 | | ASN A 367 | 187.348 1 | | | | A | C |
| ATOM | | | | | | | | A | Ö |
| ATOM | 2020 | | ASN A 367 | 186.644 1 | | | | | |
| MOTA | 2021 | | PRO A 368 | 187.174 1 | | | | A | N |
| ATOM | 2022 | CD | PRO A 368 | 187.763 1 | | | | A | С |
| ATOM | 2023 | | PRO A 368 | 186.181 1 | 169.073 | -12.682 | 1.00 21.45 | A | С |
| | ~ | | | | | | | | |

65/73

| ATOM | 2024 | CB | PRO | Δ | 368 | | 186 29 | 2 | 170 571 | -12.377 | 1 00 | | | _ |
|------|------|-----|------|----|-----|---|-----------------|-----|-----------------|---------|------|-------|----|---|
| | | | | | | | 100.23 | | 170.571 | -12.3// | 1.00 | 23.08 | A | С |
| ATOM | 2025 | CG | PRO | A | 368 | | 187.70 | 5 | 170.942 | -12.864 | 1.00 | 19.70 | A | C |
| ATOM | 2026 | С | PRO | Α | 368 | | 184.75 | 5 | 168.638 | -13.047 | 1 00 | 22.70 | Α | C |
| ATOM | 2027 | 0 | | | 368 | | | | | -12.209 | | | | |
| | | | | | | • | TO4.0T(| О, | 100.091 | -12.209 | 1.00 | 21.09 | Α | 0 |
| MOTA | 2028 | N | SER | Α | 369 | | 184.386 | 6 | 168.865 | -14.303 | 1.00 | 21.10 | Α | N |
| ATOM | 2029 | CA | SER | А | 369 | | 183.069 | 8 | 168.492 | -14.818 | | 25.15 | | С |
| | | | | | | | 100 01 | ~ | 160.152 | 74.010 | | | A | |
| MOTA | 2030 | CB | SER | A | 369 | | | | | -16.263 | 1.00 | 25.61 | Α | С |
| MOTA | 2031 | OG | SER | Α | 369 | | 183.11! | 5 | 170.391 | -16.341 | 1.00 | 37.93 | A | 0 |
| ATOM | 2032 | С | | | 369 | | | | | -14.785 | | | | |
| | | | | | | | | | | | 1.00 | 23.28 | A | С |
| ATOM | 2033 | 0 | SER | Α | 369 | | 181.68! | 5 : | 166.555 | -14.591 | 1.00 | 26.91 | Α | 0 |
| ATOM | 2034 | N | GT.N | ΖΔ | 370 | | | | | -14.995 | | 20.71 | | |
| | | | | | | | | | | | | | A | N |
| MOTA | 2035 | CA | GTN | Α | 370 | | 183.74 | 4 ; | 164.749 | -15.009 | 1.00 | 21.53 | A | С |
| ATOM | 2036 | CB | GLN | Α | 370 | | 184.923 | 2 | 164.172 | -15.785 | 1 00 | 24.23 | Α | C |
| ATOM | 2037 | CG | | | 370 | | | | | -17.279 | | | | |
| | | | | | | | | | | | 1.00 | 31.18 | Α | С |
| ATOM | 2038 | CD | GLN | Α | 370 | | 185.948 | 8 . | 164.183 | -18.045 | 1.00 | 38.83 | A | C |
| ATOM | 2039 | OE1 | GLN | Α | 370 | | 186.879 | 9 | 163.380 | -17.767 | 1 00 | 41.58 | A | 0 |
| | 2040 | | GLN | | | | | | | | | | | |
| MOTA | | | | | | | | | | -19.038 | 1.00 | 43.83 | Α | N |
| ATOM | 2041 | С | GLN | Α | 370 | | 183.68 | 8 : | 164.073 | -13.665 | 1.00 | 20.69 | Α | С |
| ATOM | 2042 | 0 | CT.N | Δ | 370 | | | | | -13.600 | | | | |
| | | | | | | | | | | | | 19.42 | A | 0 |
| ATOM | 2043 | N | ARG | A | 371 | | | | | -12.585 | 1.00 | 18.88 | A | N |
| ATOM | 2044 | CA | ARG | Α | 371 | | 183.90 | 6 | 164.189 | -11.252 | 1.00 | 21.24 | A | С |
| ATOM | 2045 | СВ | | | 371 | | | | | -10.231 | | | | |
| | | | | | | | | | | | | 17.55 | A | С |
| ATOM | 2046 | CG | ARG | Α | 371 | | 186.104 | 4 : | 165.158 | -10.394 | 1.00 | 15.36 | A | С |
| ATOM | 2047 | CD | ARG | А | 371 | | | | 166.286 | -9.564 | | 11.86 | | C |
| | | | | | | | | | | | | | A | |
| ATOM | 2048 | NE | | | 371 | | 18/.91 | 3. | 166./39 | -10.108 | 1.00 | 12.57 | A | N |
| ATOM | 2049 | CZ | ARG | Α | 371 | | 188.440 | 0 : | 167.951 | -9.938 | 1.00 | 14.14 | A | С |
| ATOM | 2050 | NH1 | ARG | Δ | 371 | | | | 168.878 | | | | | |
| | | | | | | | | | | -9.216 | | 10.91 | A | N |
| ATOM | 2051 | NHZ | ARG | Α | 371 | | 189.583 | 3 : | 168.257 | -10.545 | 1.00 | 9.48 | Α | N |
| ATOM | 2052 | С | ARG | Α | 371 | | 182.440 | 0 : | 164.038 | -10.854 | 1 00 | 22.37 | A | С |
| ATOM | 2053 | 0 | | | 371 | | | | | -11.176 | | | | |
| | | | | | | | | | | | 1.00 | 22.50 | Α | 0 |
| MOTA | 2054 | N | PRO | Α | 372 | ; | 182.14] | 1 : | 162.957 | -10.111 | 1.00 | 23.64 | Α | N |
| ATOM | 2055 | CD | PRO | A | 372 | | 183.165 | 5 | 162.051 | -9.512 | 1 00 | 23.75 | A | C |
| | | | | | | | | | | | | | | |
| ATOM | 2056 | CA | | | 372 | | | | 162.663 | -9.653 | 1.00 | 21.80 | A | С |
| ATOM | 2057 | CB | PRO | A | 372 | | 180.923 | 3 : | 161.269 | -9.007 | 1.00 | 22.29 | A | С |
| ATOM | 2058 | CG | PRO | Δ | 372 | | | | 161.227 | -8.548 | | | | |
| | | | | | | | | | | | | 22.92 | A | С |
| MOTA | 2059 | С | PRO | А | 372 | | | | 163.726 | -8.739 | 1.00 | 21.72 | Α | С |
| ATOM | 2060 | 0 | PRO | Α | 372 | | 180.875 | 5 3 | 164.579 | -8.217 | 1.00 | 23.11 | A | 0 |
| MOTA | 2061 | N | | | 373 | | | | 163.740 | | | | | |
| | | | | | | | | | | -8.654 | 1.00 | 20.67 | A | N |
| ATOM | 2062 | CA | MET | A | 373 | | 178.153 | 3 | 164.668 | -7.731 | 1.00 | 19.68 | A | С |
| MOTA | 2063 | CB | MET | Α | 373 | | 176.674 | 4 : | 164.841 | -8.137 | 1 00 | 25.32 | A | С |
| MOTA | 2064 | CG | | | 373 | | | | | | | | | |
| | | | | | | | | | 165.598 | -9.397 | 1.00 | 29.58 | A | С |
| ATOM | 2065 | SD | MET | Ą | 373 | | 177.27 <i>4</i> | 4] | 167.224 | -9.216 | 1.00 | 44.08 | Α | S |
| ATOM | 2066 | CE | MET | Α | 373 | | 175.850 | n 1 | 168.314 | -8.571 | 1 00 | 34.35 | A | C |
| ATOM | 2067 | C | | | 373 | | | | | | | | | |
| | | | | | | | | | 163.942 | -6.368 | 1.00 | 18.77 | A | С |
| MOTA | 2068 | 0 | MET | Α | 373 | | 178.518 | B 1 | 162.750 | -6.337 | 1.00 | 14.31 | A | 0 |
| MOTA | 2069 | N | UHJ | А | 374 | | 177 985 | 5 1 | 164.639 | -5.257 | | 16.82 | | |
| | 2070 | | | | | | | | | | | | A | N |
| ATOM | | CA | | | 374 | | | | 163.984 | -3.959 | 1.00 | 17.05 | A | С |
| ATOM | 2071 | CB | LEU | Α | 374 | - | 177.959 | 9 1 | 165.010 | -2.820 | 1.00 | 15.61 | A | C |
| MOTA | 2072 | CG | LEU | Δ | 374 | | | | 165.888 | -2.751 | | 17.98 | | |
| | | | LEU | | | | | | | | | | A | С |
| MOTA | 2073 | | | | | | | | 167.269 | -2.145 | 1.00 | | A | С |
| ATOM | 2074 | CD2 | LEU | А | 374 | 1 | 180.290 | 0 1 | 165.125 | -1.973 | 1.00 | 12.26 | Α | С |
| ATOM | 2075 | С | LEU | Δ | 374 | | | | 162.915 | -3.837 | | 18.65 | | |
| | | | | | | | | | | | | | A | С |
| ATOM | 2076 | 0 | LEU | A | 3/4 | _ | 177.122 | 2] | 161.885 | -3.201 | 1.00 | 19.21 | A. | 0 |
| MOTA | 2077 | N | ARG | А | 375 | 1 | L75.804 | 4 1 | 163.167 | -4.504 | 1.00 | 18.78 | A | N |
| ATOM | 2078 | CA | ARG | | | | | | 162.248 | -4.510 | | | | |
| | | | | | | | | | | | | 20.13 | A | С |
| ATOM | 2079 | CB | ARG | A | 3/5 |] | 173.504 | 1] | L62.813 | -5.210 | 1.00 | 21.87 | Α | С |
| ATOM | 2080 | С | ARG | А | 375 | 1 | 175.033 | 3 1 | 160.942 | -5.178 | 1.00 | 21.00 | A | C |
| ATOM | 2081 | 0 | ARG | | | | | | | | | | | |
| | | | | | | | | | L59.916 | -4.909 | | 21.05 | A | 0 |
| MOTA | 2082 | N | GLU | A | 376 | 3 | L75.970 |) 1 | L61.009 | -6.106 | 1.00 | 23.11 | Α | N |
| ATOM | 2083 | CA | GLU | A | 376 | 1 | 76.419 | 9 1 | 159.788 | -6.763 | | 23.55 | A | |
| ATOM | 2084 | СВ | GLU | | | | | | | | | | | C |
| | | | | | | | | | 160.139 | -8.053 | | 24.82 | A | С |
| ATOM | 2085 | CG | GLU | Α | 376 | 1 | .76.400 |) 1 | L 61.110 | -8.977 | 1.00 | 32.25 | A | С |
| ATOM | 2086 | CD | GLU | | | | | | | -10.206 | | 34.95 | | |
| | | | | | | | | | | | | | A | С |
| MOTA | 2087 | | GLU | | | | | | | -10.770 | 1.00 | 37.06 | Α | 0 |
| ATOM | 2088 | OE2 | GLU | Α | 376 | 1 | .78.110 |) 1 | .60.783 | -10.630 | | 37.87 | A | ō |
| ATOM | 2089 | С | GLU | | | | | | 58.962 | | | | | |
| | | | | | | | | | | -5.852 | | 23.36 | A | С |
| ATOM | 2090 | 0 | GLU | A | 376 | 1 | .//.448 | 1 | .57.712 | -5.874 | 1.00 | 25.32 | A | 0 |
| ATOM | 2091 | N | VAL | А | 377 | 1 | 78.204 | 1 | .59.683 | -5.113 | | 20.65 | A | N |
| ATOM | 2092 | | | | | | | | | | | | | |
| | | CA | VAL | | | | | | .59.065 | -4.241 | | 19.06 | A | С |
| ATOM | 2093 | CB | VAL | A | 377 | 1 | .80.021 | . 1 | .60.117 | -3.550 | 1.00 | 20.25 | A | С |
| | | | | | | | | | | | | | | - |

| ATOM | 2094 | CGI | VAL | Α | 377 | 180.772 | 159.513 | -2.415 | 100 | 14.07 | | A | С |
|--------------|--------------|----------|------------|---|------------|---------|--------------------|------------------|------|----------------|---|--------|--------|
| ATOM | 2095 | | VAL | | | | 160.762 | -4.587 | | 16.78 | | A | c |
| MOTA | 2096 | С | VAL | A | 377 | | 158.284 | -3.229 | | 20.23 | | A | Č |
| MOTA | 2097 | 0 | VAL | A | 377 | | 157.099 | -3.037 | | 20.59 | | A | ō |
| ATOM | 2098 | N | LEU | Α | 378 | 177.392 | 158.937 | -2.620 | 1.00 | 20.07 | | A | N |
| MOTA | 2099 | CA | LEU | Α | 378 | 176.526 | 158.314 | -1.619 | 1.00 | 20.48 | | A | С |
| MOTA | 2100 | CB | LEU | Α | 378 | 175.514 | 159.346 | -1.107 | 1.00 | 19.33 | | A | С |
| ATOM | 2101 | CG | | | 378 | | 160.087 | 0.237 | 1.00 | 25.33 | | A | С |
| ATOM | 2102 | | LEU | | | 177.197 | 159.794 | 0.722 | 1.00 | 23.60 | | A | С |
| ATOM | 2103 | | LEU | | | | 161.610 | 0.073 | 1.00 | 20.05 | | Α | С |
| MOTA | 2104 | С | | | 378 | | 157.030 | -2.120 | | 22.64 | | A | С |
| MOTA | 2105 | 0 | | - | 378 | | 156.130 | -1.318 | | 21.93 | | A | 0 |
| ATOM | 2106 | N | | | 379 | | 156.930 | -3.435 | | 19.85 | | A | N |
| ATOM | 2107 | CA | | | 379 | | 155.756 | -4.020 | | 24.21 | | A | С |
| ATOM | 2108 | CB | | | 379 | | 156.118 | -5.171 | | 29.18 | | A | C |
| ATOM ATOM | 2109 2110 | CG CD | | | 379 379 | | 157.140 | -4.872 | | 37.87 | | A | C |
| ATOM | 2111 | OE1 | | | 379 | | 157.458 157.586 | -6.104 -7.214 | | 44.63 | | A. | C |
| ATOM | 2112 | OE2 | | | | | 157.587 | -5.961 | | 47.26 46.30 | | A A | 0 |
| ATOM | 2113 | C | | | 379 | | 154.817 | -4.623 | | 22.35 | | A | 0 |
| ATOM | 2114 | ŏ | | | 379 | | 153.788 | -5.180 | | 22.07 | | A | 0 |
| ATOM | 2115 | N | | | 380 | | 155.165 | -4.555 | | 20.53 | | A | N |
| ATOM | 2116 | CA | | | 380 | | 154.301 | -5.145 | | 20.63 | | A | C |
| ATOM | 2117 | СВ | | | 380 | | 154.909 | -4.995 | | 15.41 | | A | č |
| ATOM | 2118 | CG | HIS | Α | 380 | | 154.184 | -5.800 | | 17.05 | | A | č |
| MOTA | 2119 | CD2 | HIS | Α | 380 | | 154.493 | -6.982 | | 16.91 | | A | С |
| MOTA | 2120 | ND1 | HIS | A | 380 | 181.129 | 152.901 | -5.498 | 1.00 | 16.78 | | A | N |
| MOTA | 2121 | | HIS | | | | 152.453 | -6.459 | 1.00 | 16.66 | | A | С |
| MOTA | 2122 | | HIS | | | 182.042 | 153.399 | -7.372 | | 15.37 | | A | N |
| ATOM | 2123 | C | | | 380 | | 152.904 | -4.509 | | 20.19 | | A | С |
| ATOM | 2124 | 0 | | | 380 | | 152.774 | -3.293 | | 21.40 | | A | 0 |
| ATOM | 2125 | N | | | 381 | | 151.843 | -5.333 | | 21.11 | | A | N |
| ATOM | 2126 2127 | CD | | | 381 | | 151.912 | -6.792 | | 20.62 | | A | C |
| ATOM ATOM | 2127 | CA CB | | | 381 381 | | 150.440 149.635 | -4.874 | | 22.07 | | A | C |
| ATOM | 2129 | CG | | | 381 | | 150.510 | -6.139 -7.246 | | 23.24 | | A | C |
| ATOM | 2130 | C | | | 381 | | 150.109 | -3.708 | | 25.34 20.71 | | A A | C |
| ATOM | 2131 | ŏ | | | 381 | | 149.416 | -2.762 | | 22.12 | | A A | 0 |
| ATOM | 2132 | N | | | 382 | | 150.607 | -3.783 | | 19.08 | | A | И |
| ATOM | 2133 | CA | | | 382 | | 150.367 | -2.733 | | 18.09 | | A | C |
| ATOM | 2134 | CB | TRP | Α | 382 | | 150.885 | -3.160 | | 16.26 | | A | č |
| ATOM | 2135 | CG | TRP | Α | 382 | 183.757 | 150.595 | -2.180 | 1.00 | 17.75 | | A | Ċ |
| MOTA | 2136 | CD2 | TRP | Α | 382 | 184.370 | 151.524 | -1.271 | 1.00 | 17.24 | | A | C |
| MOTA | 2137 | CE2 | | | 382 | 185.366 | 150.816 | -0.559 | 1.00 | 16.47 | | A | С |
| ATOM | 2138 | CE3 | | | 382 | | 152.882 | -0.983 | 1.00 | 17.55 | | A | C |
| ATOM | 2139 | CD1 | | | | | 149.398 | -1.986 | | 14.76 | | A | С |
| ATOM | 2140 | | TRP | | | | 149.524 | -1.022 | | 16.65 | | A | N |
| ATOM | 2141 | | TRP | | | | 151.422 | 0.421 | | 15.85 | | A | С |
| ATOM | 2142 2143 | | TRP TRP | | | | 153.487 | -0.002 | | 19.06 | | A | С |
| ATOM ATOM | 2143 | Cnz | TRP | | | | 152.754 151.042 | 0.687 | | 17.35 | | A | C |
| ATOM | 2145 | 0 | TRP | | | | 150.467 | -1.431 -0.352 | | 18.11 19.08 | | A. | C |
| ATOM | 2146 | N | | | 383 | | 152.266 | -1.533 | | 18.03 | | A. | 0 |
| ATOM | 2147 | CA | | | 383 | | 153.003 | -0.354 | | 17.34 | | A A | N C |
| ATOM | 2148 | СВ | ILE | | | | 154.460 | -0.709 | | 15.70 | | A | C |
| ATOM | 2149 | | ILE | | | | 155.178 | 0.495 | | 13.48 | | A | C |
| ATOM | 2150 | CG1 | ILE | Α | 383 | | 155.212 | -1.132 | 1.00 | 8.79 | | A | Č |
| ATOM | 2151 | CD1 | ILE | Α | 383 | | 155.455 | 0.019 | | 11.19 | | A. | č |
| ATOM | 2152 | С | ILE | Α | 383 | 178.790 | 152.312 | 0.324 | | 19.72 | | A | Ċ |
| ATOM | 2153 | 0 | ILE | Α | 383 | 178.851 | 152.044 | 1.523 | 1.00 | 21.11 | | A | 0 |
| ATOM | 2154 | N | THR | | | | 151.994 | -0.428 | 1.00 | 18.67 | | A | N |
| ATOM | 2155 | CA | THR | | | | 151.336 | 0.180 | | 21.04 | | A | C |
| ATOM | 2156 | СВ | THR | | | | 151.287 | -0.784 | 1.00 | 22.27 | | A | С |
| ATOM | 2157 | OG1 | | | | 175.657 | | -1.912 | | 23.10 | | A | 0 |
| ATOM | 2158 | | THR | | | | 152.706 | -1.271 | | 15.14 | | A | С |
| ATOM | 2159 | C | THR | | | | 149.921 | 0.721 | | 20.77 | | A | С |
| ATOM | 2160 | 0 | THR | | | | 149.496 | 1.683 | | 24.40 | | A | 0 |
| ATOM | 2161 | N | ALA | | | | 149.206 | 0.138 | | 18.85 | | A. | N |
| ATOM | 2162 | CA | ALA | | | 178.195 | | 0.598 | | 16.58 | | A. | C |
| ATOM | 2163 | СВ | ALA | A | 202 | 178.996 | 141.119 | -0.481 | 1.00 | 8.89 | - | A. | С |
| | | | | | | | | | | | | | |

| ATOM | 2164 | С | ALA | A | 385 | 179.021 | 147.877 | 1.890 | 1.00 19.30 | A | С |
|--------------|--------------|-----------|------------|---|----------|---------|--------------------|------------------|--------------------------|--------|--------|
| ATOM | 2165 | 0 | ALA | Α | 385 | 178.987 | 146.950 | 2.699 | 1.00 17.69 | A | 0 |
| ATOM | 2166 | N | ASN | | | | 148.966 | 2.104 | 1.00 23.78 | A | N |
| MOTA | 2167 | CA | ASN | | | | 149.059 | 3.274 | 1.00 24.44 | A | С |
| MOTA | 2168 | CB | ASN | | | | 149.240 | 2.783 | 1.00 22.82 | A | C |
| MOTA | 2169 | CG | ASN | | | | 148.051 | 1.997 | 1.00 22.92 | A | C |
| ATOM | 2170 | | ASN | | | | 146.947 | 2.539 | 1.00 23.56 | A | 0 |
| ATOM | 2171 2172 | C | ASN ASN | | | | 148.251 150.133 | 0.706 4.291 | 1.00 20.68 1.00 25.32 | A A | N C |
| MOTA MOTA | 2172 | 0 | ASN | | | | 150.133 | 5.366 | 1.00 25.70 | A | 0 |
| ATOM | 2174 | N | SER | | | | 151.009 | 3.950 | 1.00 28.67 | A | N |
| ATOM | 2175 | CA | SER | | | | 152.111 | 4.823 | 1.00 30.65 | A | C |
| ATOM | 2176 | СВ | | | 387 | | 153.232 | 3.955 | 1.00 29.51 | A | Ċ |
| ATOM | 2177 | OG | | | 387 | 178.208 | 154.364 | 4.724 | 1.00 35.78 | A | 0 |
| MOTA | 2178 | С | | | 387 | 178.063 | 151.687 | 5.890 | 1.00 32.67 | A | С |
| MOTA | 2179 | 0 | SER | A | 387 | 177.162 | 150.889 | 5.535 | 1.00 35.02 | A | 0 |
| ATOM | 2180 | OXT | SER | Α | 387 | | 152.164 | 7.055 | 1.00 35.90 | A | 0 |
| ATOM . | 2181 | СВ | SER | | 7 | | 195.899 | 10.921 | 1.00 30.72 | В | С |
| MOTA | 2182 | OG | SER | | 7 | | 195.490 | 11.062 | 1.00 28.92 | В | 0 |
| ATOM | 2183 | C | SER | | 7 | | 193.792 | 12.227 | 1.00 32.69 | В | C |
| MOTA | 2184 | 0 | SER | | 7 | | 192.918 195.368 | 11.331 | 1.00 33.35 | В | 0 |
| ATOM ATOM | 2185 2186 | N CA | SER SER | | 7 7 | | 195.268 | 11.576 12.001 | 1.00 34.34 1.00 32.37 | B B | N C |
| ATOM | 2186 | N | TYR | | 8 | | 193.527 | 13.402 | 1.00 32.37 | В | N |
| ATOM | 2188 | CA | TYR | | 8 | | 192.188 | 13.775 | 1.00 25.10 | В | c |
| ATOM | 2189 | СВ | TYR | | 8 | | 191.681 | 14.999 | 1.00 22.64 | В | č |
| ATOM | 2190 | CG | TYR | | 8 | | 191.579 | 14.731 | 1.00 22.03 | В | C |
| MOTA | 2191 | CD1 | TYR | В | 8 | 189.806 | 192.667 | 14.982 | 1.00 19.79 | В | С |
| ATOM | 2192 | CE1 | TYR | В | 8 | 191.153 | 192.623 | 14.642 | 1.00 19.33 | В | C |
| ATOM | 2193 | | TYR | | 8 | | 190.435 | 14.128 | 1.00 18.09 | В | С |
| MOTA | 2194 | | TYR | | 8 | | 190.391 | 13.775 | 1.00 18.91 | В | С |
| MOTA | 2195 | CZ | TYR | | | • | 191.488 | 14.038 | 1.00 20.94 | В | С |
| ATOM | 2196 | ОН | TYR | | | | 191.444 | 13.712 | 1.00 23.31 | В | 0 |
| MOTA | 2197 | C | TYR | | | | 192.143 191.422 | 14.045 14.936 | 1.00 24.33 1.00 23.49 | B B | С |
| ATOM ATOM | 2198 2199 | N O | TYR SER | | | | 192.931 | 13.263 | 1.00 23.49 | В | O N |
| ATOM | 2200 | CA | SER | | | | 193.017 | 13.314 | 1.00 24.45 | В | C |
| ATOM | 2201 | CB | SER | | | | 194.444 | 13.006 | 1.00 23.56 | В | č |
| ATOM | 2202 | ŌĞ | SER | | | | 195.336 | 14.059 | 1.00 29.98 | В | ō |
| MOTA | 2203 | С | SER | В | 9 | 182.426 | 192.085 | 12.229 | 1.00 22.36 | В | C |
| MOTA | 2204 | 0 | SER | В | 9 | 182.469 | 192.408 | 11.035 | 1.00 22.10 | В | 0 |
| MOTA | 2205 | N | TYR | | | | 190.938 | 12.653 | 1.00 20.97 | В | N |
| MOTA | 2206 | CA | TYR | | 10 | | 189.932 | 11.728 | 1.00 21.80 | В | С |
| ATOM | 2207 | CB | TYR | | | | 188.582 | 12.063 | 1.00 21.23 | В | C |
| ATOM | 2208 2209 | CG CD1 | TYR TYR | | 10 10 | | 188.617 187.694 | 12.082 12.836 | 1.00 23.30 | B B | C |
| ATOM ATOM | 2210 | | TYR | | | | 187.683 | 12.816 | 1.00 24.95 1.00 25.40 | В | C |
| ATOM | 2211 | | TYR | | | | 189.542 | 11.311 | 1.00 23.40 | В | c |
| ATOM | 2212 | | TYR | | | | 189.541 | 11.285 | 1.00 24.34 | В | č |
| ATOM | 2213 | CZ | TYR | | | | 188.600 | 12.036 | 1.00 26.19 | В | C |
| ATOM | 2214 | OH | TYR | В | 10 | 187.800 | 188.526 | 11.956 | 1.00 31.92 | В | 0 |
| MOTA | 2215 | C | TYR | | | 179.918 | 189.807 | 11.832 | 1.00 21.84 | В | C |
| MOTA | 2216 | 0 | TYR | | | | 190.098 | 12.872 | 1.00 22.91 | В | 0 |
| MOTA | 2217 | N | ASP | | | | 189.372 | 10.754 | 1.00 19.80 | В | N |
| ATOM | 2218 | CA | ASP | | | | 189.173 | 10.751 | 1.00 19.63 | В | C |
| ATOM | 2219 2220 | CB CG | ASP ASP | | | | 189.274 189.141 | 9.310 9.217 | 1.00 21.09 1.00 23.91 | В | C |
| ATOM ATOM | 2221 | | ASP | | | | 188.957 | 10.256 | 1.00 23.91 | B B | C 0 |
| ATOM | 2222 | | ASP | | | | 189.221 | 8.077 | 1.00 22.90 | В | Ö |
| ATOM | 2223 | C | ASP | | | | 187.756 | 11,297 | 1.00 19.67 | В | c |
| ATOM | 2224 | ō | ASP | | | | 186.820 | 10.565 | 1.00 20.37 | В | ō |
| ATOM | 2225 | N | ALA | | | 177.844 | 187.593 | 12.590 | 1.00 19.26 | В | N |
| MOTA | 2226 | CA | ALA | В | 12 | | 186.285 | 13.174 | 1.00 19.72 | В | С |
| MOTA | 2227 | CB | ALA | | | | 185.498 | 13.013 | 1.00 20.60 | В | С |
| ATOM | 2228 | C | ALA | | | | 186.502 | 14.640 | 1.00 20.60 | В | С |
| ATOM | 2229 | 0 | ALA | | | | 187.632 | 15.149 | 1.00 20.41 | В | 0 |
| ATOM | 2230 | И | PRO | | | | 185.448 | 15.350 | 1.00 20.13 | В | N |
| ATOM | 2231 | CD | PRO | | | | 184.055 185.608 | 14.907 16.761 | 1.00 17.56 1.00 16.88 | B B | C |
| ATOM ATOM | 2232 2233 | CA CB | PRO PRO | | | | 184.246 | 17.137 | 1.00 16.88 | В | С |
| VI ON | 2233 | ÇD | FRU | 0 | 10 | 1,0.709 | -01.240 | ± , . ± 5 , | 1.00 10.20 | 2 | C |

| MOTA | 2234 | CG | PRO | В | 13 | 175.670 | 183.563 | 15.811 | 1.00 18.64 | В | С |
|--------------|--------------|----------|------------|---|----------|--------------------|--------------------|------------------|--------------------------|--------|--------|
| MOTA | 2235 | C | PRO | | 13 | | 186.014 | 17.728 | 1.00 17.09 | В | С |
| MOTA | 2236 | 0 | PRO | | 13 | | 185.573 | 17.590 | 1.00 17.90 | В | 0 |
| ATOM | 2237 | N | SER | | 14 | | 186.839 | 18.720 | 1.00 17.14 | В | N |
| ATOM ATOM | 2238 2239 | CA CB | SER | | 14 14 | | 187.258 188.499 | 19.739 19.294 | 1.00 20.00 | В | C |
| ATOM | 2240 | OG | SER | | 14 | | 189.384 | 18.544 | 1.00 19.42 1.00 30.47 | B B | С 0 |
| ATOM | 2241 | C | SER | | 14 | | 187.518 | 21.069 | 1.00 18.32 | В | c |
| MOTA | 2242 | 0 | SER | В | 14 | | 187.968 | 22.056 | 1.00 14.51 | В | ō |
| MOTA | 2243 | N | ASP | | 15 | | 187.215 | 21.076 | 1.00 18.48 | В | N |
| MOTA | 2244 | CA | ASP | | 15 | | 187.376 | 22.248 | 1.00 23.79 | В | С |
| MOTA | 2245 2246 | CB | ASP | | 15 15 | | 187.526 | 21.783 | 1.00 30.49 | В | C |
| ATOM ATOM | 2240 | CG | ASP ASP | | 15 | | 188.932 189.605 | 21.226 20.616 | 1.00 39.83 1.00 44.43 | В | C |
| ATOM | 2248 | | ASP | | 15 | | 189.378 | 21.401 | 1.00 45.45 | B B | 0 |
| ATOM | 2249 | С | ASP | | 15 | | 186.172 | 23.199 | 1.00 21.79 | В | c |
| ATOM | 2250 | 0 | ASP | В | 15 | | 185.035 | 22.754 | 1.00 22.39 | В | 0 |
| MOTA | 2251 | N | PHE | | 16 | | 186.432 | 24.500 | 1.00 21.47 | В | N |
| ATOM | 2252 | CA | PHE | | 16 | | 185.373 | 25.514 | 1.00 22.21 | В | C |
| ATOM ATOM | 2253 2254 | CB CG | PHE PHE | | 16 16 | | 185.993 184.978 | 26.930 28.025 | 1.00 19.46 1.00 18.34 | В | C |
| ATOM | 2255 | CD1 | | | 16 | | 184.362 | 28.491 | 1.00 18.34 | B B | C |
| ATOM | 2256 | | PHE | | 16 | | 184.569 | 28.528 | 1.00 15.51 | В | C |
| MOTA | 2257 | CE1 | PHE | В | 16 | 176.716 | 183.339 | 29.435 | 1.00 18.59 | В | Ċ |
| ATOM | 2258 | | PHE | | 16 | | 183.552 | 29.469 | 1.00 15.01 | В | C |
| ATOM | 2259 | CZ | PHE | | 16 | | 182.939 | 29.921 | 1.00 15.05 | В | С |
| ATOM ATOM | 2260 2261 | 0 | PHE PHE | | 16 16 | | 184.448 184.938 | 25.301 25.058 | 1.00 21.16 | В | C |
| ATOM | 2262 | N | ILE | | 17 | | 183.135 | 25.370 | 1.00 21.78 1.00 19.97 | B B | O N |
| ATOM | 2263 | CA | ILE | | 17 | | 182.163 | 25.182 | 1.00 20.86 | В | C |
| MOTA | 2264 | CB | ILE | В | 17 | | 181.144 | 24.009 | 1.00 21.47 | В | Ċ |
| ATOM | 2265 | CG2 | | | 17 | | 179.964 | 24.011 | 1.00 11.76 | В | С |
| MOTA | 2266 | CG1 | ILE | | 17 | | 181.844 | 22.654 | 1.00 16.04 | В | С |
| ATOM ATOM | 2267 2268 | CD1 | ILE ILE | | 17 17 | | 181.051 181.318 | 21.631 26.439 | 1.00 18.42 | В | C |
| ATOM | 2269 | õ | ILE | | 17 | | 180.965 | 27.086 | 1.00 21.56 1.00 23.11 | B B | C |
| MOTA | 2270 | N | ASN | | 18 | | 181.002 | 26.778 | 1.00 24.87 | В | И |
| ATOM | 2271 | CA | ASN | В | 18 | 171.893 | 180.143 | 27.928 | 1.00 26.79 | В | C. |
| ATOM | 2272 | CB | ASN | | 18 | | 180.437 | 28.427 | 1.00 26.34 | В | С |
| ATOM | 2273 | CG | ASN | | 18 | 170.052 | 179.482 | 29.543 | 1.00 30.28 | В | С |
| ATOM ATOM | 2274 2275 | | ASN ASN | | 18 18 | | 178.519 179.747 | 29.870 30.125 | 1.00 30.01 | В | 0 |
| ATOM | 2276 | C | ASN | | 18 | | 178.718 | 27.373 | 1.00 28.50 1.00 28.06 | B B | N C |
| MOTA | 2277 | 0 | ASN | | 18 | 170.947 | | 26.737 | 1.00 31.09 | В | ő |
| MOTA | 2278 | N | PHE | | 19 | 172.969 | | 27.616 | 1.00 30.32 | В | N |
| MOTA | 2279 | CA | PHE | | 19 | 173.027 | | 27.050 | 1.00 32.46 | В | С |
| ATOM ATOM | 2280 2281 | CB CG | PHE PHE | | 19 19 | 174.460 175.430 | | 27.076 | 1.00 27.50 | B | C |
| ATOM | 2282 | | PHE | | 19 | 176.332 | | 26.214 26.785 | 1.00 22.59 1.00 20.42 | B B | C |
| ATOM | 2283 | | PHE | | 19 | 175.426 | | 24.831 | 1.00 20.42 | В | C |
| ATOM | 2284 | | PHE | | 19 | 177.223 | 178.454 | 25.989 | 1.00 19.77 | В | Č |
| ATOM | 2285 | | PHE | | 19 | 176.312 | | 24.021 | 1.00 18.13 | В | C |
| ATOM | 2286 | CZ | PHE | | 19 | 177.206 | | 24.605 | 1.00 19.50 | В | С |
| ATOM ATOM | 2287 2288 | С 0 | PHE PHE | | 19 19 | 172.086 172.063 | | 27.618 27.124 | 1.00 36.90 1.00 41.31 | В | C |
| ATOM | 2289 | N | SER | | 20 | 171.317 | | 28.646 | 1.00 41.31 | B B | O N |
| ATOM | 2290 | CA | SER | | 20 | 170.402 | | 29.142 | 1.00 46.46 | В | C |
| MOTA | 2291 | CB | SER | | 20 | 170.317 | | 30.652 | 1.00 47.60 | В | Ċ |
| MOTA | 2292 | OG | SER | | 20 | 170.456 | | 31.032 | 1.00 49.62 | В | 0 |
| ATOM ATOM | 2293 2294 | С О | SER SER | | 20 20 | 169.029 168.337 | | 28.496 | 1.00 48.43 | В | C |
| ATOM | 2295 | N | SER | | 21 | 168.645 | | 28.170 28.286 | 1.00 50.43 1.00 50.08 | В | 0 |
| ATOM | 2296 | CA | SER | | 21 | 167.349 | | 27.676 | 1.00 50.65 | B B | N C |
| ATOM | 2297 | СВ | SER | | 21 | 166.742 | | 28.317 | 1.00 49.82 | В | C |
| MOTA | 2298 | OG | SER | | 21 | 167.467 | | 27.866 | 1.00 50.01 | В | ō |
| ATOM | 2299 | C | SER | | 21 | 167.581 | | 26.204 | 1.00 51.89 | В | C |
| ATOM ATOM | 2300 2301 | O OXT | SER SER | | 21 21 | 166.843 | | 25.325 | 1.00 51.53 | В | 0 |
| ATOM | 2302 | CB | ASN | | 30 | 168.482 165.336 | | 25.953 10.155 | 1.00 53.54 1.00 41.18 | B C | 0 |
| ATOM | 2303 | CG | ASN | | 30 | 164.486 | | 9.178 | 1.00 46.58 | C | C |
| | | | - | | - | | | | | ~ | _ |

49.62

...,40 1.00 49.11

10.314 1.00 36.00

...,202 179.731 9.143 1.00 34.36

165.267 179.744 11.676 1.00 37.72

166.154 178.688 11.078 1.00 38.33

168.406 179.537 11.026 1.00 32.89

169.605 180.229 10.589 1.00 28.57

170.635 180.011 11.676 1.00 31.08

171.873 180.840 11.426 1.00 30.71

169.991 180.405 13.012 1.00 34.10

169.738 181.909 13.147 1.00

170.254 180.041 8.808 1.00 49.62 8.740 1.00 49.11 MOTA 2304 OD1 ASN C 30 164.828 179.693 0 ND2 ASN C 30 MOTA 2305 N ATOM 2306 ASN C 30 С С MOTA 2307 0 ASN C 30 0 ASN C 30 ATOM 2308 N ASN C 30 ILE C 31 ILE C 31 MOTA 2309 CA С MOTA 2310 N N MOTA 2311 CA С MOTA 2312 ILE C 31 CB С С CG2 ILE C 31 MOTA 2313 С C CG1 ILE C 31 MOTA 2314 С С ILE C 31 ILE C 31 MOTA 2315 CD1 ILE C С С MOTA 2316 С С С 170.816 180.996 8.677 1.00 20.90 170.188 178.856 8.623 1.00 23.52 170.872 178.678 7.351 1.00 24.02 171.126 177.197 7.086 1.00 27.28 169.858 176.423 6.805 1.00 32.74 168.852 177.009 6.338 1.00 36.15 169.884 175.202 7.039 1.00 33.71 170.289 179.324 6.104 1.00 23.19 170.804 179.126 5.001 1.00 22.55 169.223 180.090 6.271 1.00 21.46 168.608 180.781 5.136 1.00 22.57 2317 ILE C 31 ATOM 0 С 0 MOTA 2318 N ASP C 32 С N ASP C 32 MOTA 2319 CA С C CB ASP C 32 CG ASP C 32 OD1 ASP C 32 ATOM 2320 7.086 1.00 27.28 С С 2321 ATOM С С ATOM 2322 0 ATOM 2323 OD2 ASP C 32 С 0 ATOM 2324 С ASP C 32 С С ASP C 32 SER C 33 SER C 33 MOTA 2325 0 5.001 1.00 22.55 С 0 MOTA 2326 N С N

 168.608
 180.781
 5.136
 1.00
 22.37

 167.205
 181.244
 5.499
 1.00
 23.28

 166.326
 180.142
 5.639
 1.00
 33.59

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 182.002
 4.805
 1.00
 19.49

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 1.00
 20.33

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 1.00
 18.04

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 1.00
 16.02

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 15.82

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 14.91

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 6.330
 1.00
 14.91

 176.727
 183.738
 5.538
 1.00
 10.61

 ATOM 2327 CA С С MOTA 2328 CB SER C 33 С C MOTA 2329 OG SER C 33 С 0 SER C 33 SER C 33 TRP C 34 MOTA 2330 С С 2331 ATOM 0 С O ATOM 2332 N С N MOTA 2333 CA TRP C 34 С С ATOM 2334 CB TRP C 34 С С CG TRP C 34 CD2 TRP C 34 ATOM 2335 С ATOM 2336 С С CE2 TRP C 34 ATOM 2337 С С MOTA 2338 CE3 TRP C 34 С С CD1 TRP C 34
NE1 TRP C 34
CZ2 TRP C 34 MOTA 2339 С С MOTA 2340 С 2341 MOTA С C 2342 CZ3 TRP C 34 MOTA С С MOTA 2343 CH2 TRP C 34 С С TRP C 34 TRP C 34 PHE C 35 172.022 183.499 4.299 MOTA 2344 C 1.00 15.62 С C 3.735 MOTA 2345 0 172.435 182.324 173 183 163 172.251 184.579 1.00 16.88 С 0 MOTA 2346 N 3.819 1.00 13.45 С Ν MOTA 2347 PHE C 35 173.191 182.222 2.567 CA 1.00 12.33 С С 173.191 182.222 2.567 1.00 12.33 173.739 180.801 2.344 1.00 8.78 174.597 180.304 3.456 1.00 9.30 174.042 179.566 4.495 1.00 9.43 175.960 180.610 3.500 1.00 9.38 174.822 179.141 5.565 1.00 6.69 176.749 180.190 4.569 1.00 8.62 176.174 179.455 5.602 1.00 10.55 172.367 182.623 1.351 1.00 13.51 172.779 183.502 0.597 1.00 13.63 PHE C 35 MOTA 2348 CB С С CG PHE C 35 CD1 PHE C 35 CD2 PHE C 35 ATOM 2349 С C ATOM 2350 С С MOTA 2351 С С MOTA 2352 CE1 PHE C 35 С C CE2 PHE C 35 MOTA 2353 С С PHE C 35 PHE C 35 2354 ATOM CZС C 2355 ATOM С С C PHE C 35 MOTA 2356 0 С 0 MOTA 2357 ALA C 36 171.207 181.997 1.153 N 1.00 14.52 С N CA MOTA 2358 ALA C 36 170.392 182.349 -0.008 1.00 18.05 С С ALA C 36 ALA C 36 2359 169.246 181.349 -0.209 1.00 13.28 ATOM CB С С 2360 169.844 183.775 ATOM C 0.103 1.00 18.08 С С 2361 ALA C 36 169.797 184.500 -0.899 1.00 20.25 MOTA 0 С 0 169.458 184.192 1.307 1.00 18.61 ATOM 2362 N GLU C 37 С N GLU C 37 ATOM 2363 CA 168.905 185.536 1.505 1.00 21.91 С С 2.933 1.00 22.41 2364 CB GLU C 168.391 185.686 MOTA 37 С 3.240 С 2365 GLU C ATOM CG 37 167.103 184.901 1.00 24.75 С ATOM 2366 CD GLU C 37 166.619 185.133 4.681 1.00 30.55 С С 167.473 185.511 5.529 1.00 31.00 ATOM 2367 OE1 GLU C 37 С 0 OE2 GLU C 37 2368 MOTA 165.414 184.932 4.976 1.00 30.11 С 0 GLU C ATOM 2369 С 37 169.913 186.649 1.194 1.00 22.74 С С 0.791 1.00 22.40 1.375 1.00 25.80 2370 ATOM 0 37 169.561 187.754 С LYS C 38 2371 N 171.181 186.332 ATOM С N 2372 CA LYS C MOTA 38 172.269 187.252 1.00 24.79 1.114 C 2373 CB LYS C 38 ATOM 173.438 186.831 1.982 1.00 27.15 С C

| ATOM | 2374 | CG | LYS | С | 38 | 174.708 | 187.488 | 1.649 | 1.00 | 30.16 | 1 | 2 | С |
|--------------|--------------|-----|------------|---|-----|---------|-----------|--------|------|-------|---|--------|---|
| ATOM | 2375 | CD | LYS | С | 38 | 175.776 | 187.057 | 2.622 | 1.00 | 31.96 | | 2 | С |
| ATOM | 2376 | CE | LYS | | 38 | | 187.927 | 2.391 | 1.00 | | | ā | c |
| ATOM | 2377 | NZ | LYS | | 38 | | 187.735 | 3.456 | _ | 40.31 | | C | N |
| ATOM | 2378 | C | LYS | | 38 | | 187.194 | -0.373 | | 25.05 | | C | c |
| | 2379 | Ö | LYS | | 38 | | 188.177 | | | | | | |
| ATOM | | | | | | | | -0.969 | | 23.54 | | 2 | 0 |
| MOTA | 2380 | N | ALA | | 39 | | 186.032 | -0.975 | | 23.76 | | C | N |
| ATOM | 2381 | CA | ALA | | 39 | | 185.849 | -2.400 | | 23.35 | | 2 | С |
| ATOM | 2382 | CB | ALA | | 39 | | 184.343 | -2.762 | | 20.98 | | C | С |
| MOTA | 2383 | С | ALA | | 39 | | 186.576 | -3.245 | 1.00 | 24.77 | | 2 | С |
| MOTA | 2384 | 0 | ALA | С | 39 | 171.950 | 187.112 | -4.318 | 1.00 | 24.28 | | C | 0 |
| MOTA | 2385 | N | ASN | С | 40 | 170.403 | 186.592 | -2.754 | 1.00 | 23.38 | | 3 | N |
| MOTA | 2386 | CA | ASN | С | 40 | 169.30 | 187.210 | -3.480 | 1.00 | 23.68 | | C | С |
| MOTA | 2387 | СВ | ASN | С | 40 | 167.993 | 186.526 | -3.137 | 1.00 | 18.03 | | C | С |
| MOTA | 2388 | CG | ASN | С | 40 | 168.024 | 185.035 | -3.395 | | 17.89 | | Ĉ | C |
| ATOM | 2389 | | ASN | | 40 | | 184.553 | -4.351 | | 18.06 | | Ċ. | ō |
| ATOM | 2390 | | ASN | | 40 | | 184.287 | -2.545 | | 16.76 | | c | N |
| ATOM | 2391 | C | ASN | | 40 | | 188.701 | -3.279 | | 25.17 | | c | C |
| ATOM | 2392 | Ö | ASN | | 40 | | 189.332 | -4.052 | | 27.11 | | C | 0 |
| | 2393 | N | LEU | | 41 | | 189.268 | | | | | | |
| ATOM | | | | | | | | -2.246 | | 26.95 | | C | N |
| ATOM | 2394 | CA | LEU | | 41 | | 190.709 | -1.965 | | 29.31 | | 2 | C |
| ATOM | 2395 | CB | LEU | | 41 | | 191.047 | -0.705 | | 29.88 | | C | С |
| MOTA | 2396 | CG | LEU | | 41 | | 192.308 | -0.057 | | 30.53 | | C | С |
| MOTA | 2397 | | LEU | | 41 | | 192.148 | 0.221 | 1.00 | 30.41 | | C | С |
| MOTA | 2398 | | LEU | | 41 | | 192.558 | 1.209 | 1.00 | 29.64 | | C | С |
| ATOM | 2399 | C | LEU | С | 41 | 170.09 | 191.589 | -3.120 | 1.00 | 29.84 | | C | С |
| MOTA | 2400 | 0 | LEU | С | 41 | 171.05 | 191.230 | -3.787 | 1.00 | 30.13 | | C | 0 |
| ATOM | 2401 | N | GLU | С | 42 | 169.48 | 7 192.763 | -3.312 | 1.00 | 32.17 | | C | N |
| ATOM | 2402 | CA | GLU | С | 42 | 169.85 | 193.627 | -4.439 | 1.00 | 35.33 | | C | С |
| ATOM | 2403 | CB | GLU | С | 42 | 168.583 | 3 193.847 | -5.286 | 1.00 | 33.50 | | C | С |
| ATOM | 2404 | CG | GLU | С | 42 | 167.81 | 192.560 | -5.616 | | 32.30 | | C | C |
| ATOM | 2405 | CD | GLU | | 42 | | 3 192.784 | -6.334 | | 34.80 | | Ĉ | Ċ |
| ATOM | 2406 | | GLU | | 42 | | 193.892 | -6.241 | | 34.22 | | Ċ | ō |
| ATOM | 2407 | | GLU | | 42 | | 191.829 | -6.987 | | 33.99 | | o C | o |
| ATOM | 2408 | C | GLU | | 42 | | 194.977 | -4.190 | | 37.36 | | 3 | c |
| ATOM | 2409 | ŏ | GLU | | 42 | | 195.539 | -3.109 | | | | C | |
| ATOM | 2410 | N | ASN | | 43 | | 195.457 | | | 38.22 | | | 0 |
| | | CA | | | | | | -5.221 | | 43.15 | | C C | N |
| MOTA | 2411 | | ASN | | 43 | | 196.790 | -5.266 | | 48.74 | | C | C |
| ATOM | 2412 | CB | ASN | | 43 | | 197.184 | -3.967 | | 48.84 | | 3 | C |
| MOTA | 2413 | CG | ASN | | 43 | | 196.255 | -3.632 | | 50.97 | | C | С |
| MOTA | 2414 | | ASN | | 43 | | 195.054 | -3.970 | | 50.34 | | C | 0 |
| MOTA | 2415 | | ASN | | 43 | | 3 196.804 | -2.939 | | 51.10 | | 3 | N |
| ATOM | 2416 | С | ASN | | 43 | | 196.704 | -6.455 | 1.00 | 52.67 | | 3 | С |
| MOTA | 2417 | 0 | ASN | | 43 | | 3 197.379 | -7.493 | | 54.34 | | C | 0 |
| ATOM | 2418 | OXT | ASN | | 43 | | 3 195.931 | -6.344 | 1.00 | 55.98 | 1 | 2 | 0 |
| ATOM | 2419 | PB | | | 531 | | 3 175.824 | 12.432 | | 20.87 | | S | P |
| MOTA | 2420 | O1B | ADP | S | 531 | 193.88 | 176.352 | 13.792 | 1.00 | 32.28 | | 3 | 0 |
| MOTA | 2421 | O2B | ADP | S | 531 | 193.56 | 5 176.837 | 11.394 | 1.00 | 26.12 | | S | 0 |
| ATOM | 2422 | 03B | ADP | S | 531 | 194.979 | 174.908 | 12.132 | 1.00 | 31.89 | | 3 | 0 |
| ATOM | 2423 | PA | ADP | S | 531 | 191.748 | 174.063 | 13.545 | 1.00 | 18.35 | | 3 | P |
| MOTA | 2424 | O1A | ADP | S | 531 | 190.613 | 174.901 | 14.032 | 1.00 | | | S | 0 |
| ATOM | 2425 | | ADP | | | 191.35 | 172.755 | 12.954 | 1.00 | | | | ō |
| ATOM | 2426 | | ADP | | | 192.532 | 174.874 | 12.450 | 1.00 | | | | ō |
| ATOM | 2427 | | ADP | | | | 173.906 | 14.839 | 1.00 | | | | ŏ |
| ATOM | 2428 | | ADP | | | | 172.965 | 14.869 | 1.00 | | | | č |
| ATOM | 2429 | | ADP | | | | 171.623 | 15.640 | 1.00 | | | | c |
| ATOM | 2430 | | ADP | | | | 3 171.842 | 16.897 | 1.00 | | | | |
| | | | | | | | | | | _ | | | 0 |
| ATOM ATOM | 2431 2432 | | ADP ADP | | | | 170.494 | 14.997 | 1.00 | | | | C |
| | | | | | | | 169.824 | 14.038 | 1.00 | | | | 0 |
| ATOM | 2433 | | ADP | | | | 169.659 | 16.218 | 1.00 | | | | C |
| ATOM | 2434 | | ADP | | | | 168.749 | 16.615 | 1.00 | | | | 0 |
| ATOM | 2435 | | ADP | | | | 170.704 | 17.312 | 1.00 | | | | С |
| MOTA | 2436 | N9 | ADP | | | | . 171.169 | 17.445 | 1.00 | | | | N |
| ATOM | 2437 | C8 | ADP | | | | 172.237 | 16.808 | 1.00 | 20.72 | | 3 | С |
| MOTA | 2438 | N7 | ADP | | | | 172.431 | 17.108 | 1.00 | 19.94 | 5 | 3 | N |
| ATOM | 2439 | C5 | ADP | s | 531 | 188.596 | 171.408 | 17.961 | 1.00 | 15.87 | 5 | | С |
| MOTA | 2440 | C6 | ADP | S | 531 | 187.377 | 171.071 | 18.652 | 1.00 | | | | C |
| MOTA | 2441 | N6 | ADP | | | 186.260 | 171.696 | 18.563 | 1.00 | | | | N |
| ATOM | 2442 | N1 | ADP | | | 187.474 | 169.935 | 19.454 | 1.00 | | 5 | | N |
| ATOM | 2443 | C2 | ADP | | | | 169.198 | 19.595 | 1.00 | | | | c |
| | | | | - | | | - · · · - | | | | | | - |

| | | | | _ | | 400 770 | | | | _ | ., |
|--------------|--------------|----------|------------|-----|------------|--------------------|--------------------|------------------|--------------------------|--------|--------|
| ATOM ATOM | 2444 2445 | N3 C4 | ADP ADP | S | 531 531 | 189.773 189.716 | | 18.982 18.162 | 1.00 17.25 1.00 16.09 | S S | N C |
| ATOM | 2446 | MG | MG | x | 1 | 192.801 | | 10.897 | 1.00 18.98 | x | MG+2 |
| ATOM | 2447 | MG | MG | X | 2 | 192.933 | 178.461 | 10.215 | 1.00 21.17 | Х | MG+2 |
| MOTA | 2448 | MG | MG | Х | 3 | 174.135 | 172.090 | -6.081 | 1.00 37.43 | X | MG+2 |
| MOTA | 2449 | S | SO4 | | 1 | 175.520 | 167.060 | -4.810 | 1.00 40.27 | Y Y | S |
| ATOM ATOM | 2450 2451 | 01 02 | SO4 | | 1 1 | 175.005 176.918 | 168.134 167.395 | -3.755 -5.118 | 1.00 40.61 1.00 40.85 | Y | 0 |
| ATOM | 2452 | 03 | SO4 | | ī | 175.333 | 165.874 | -4.319 | 1.00 45.29 | Y | Ö |
| ATOM | 2453 | 04 | SO4 | | 1 | 174.705 | 167.387 | -6.003 | 1.00 46.53 | Y | 0 |
| MOTA | 2454 | S | SO4 | | 2 | 196.317 | | 22.149 | 1.00 52.91 | Y | S |
| ATOM | 2455 | 01 | SO4 | | 2 | 194.902 | 160.702 | 22.904 | 1.00 53.25 | Y | 0 |
| ATOM ATOM | 2456 2457 | 02 03 | SO4 SO4 | | 2 2 | 197.156 196.808 | 161.615 159.261 | 22.484 22.506 | 1.00 52.23 1.00 50.45 | Y Y | 0 |
| ATOM | 2457 | 04 | SO4 | | 2 | 195.932 | 160.567 | 20.717 | 1.00 53.17 | Y | 0 |
| MOTA | 2459 | s | SO4 | | 3 | 184.237 | 187.281 | -0.473 | 1.00 69.64 | Ÿ | s |
| MOTA | 2460 | 01 | SO4 | Y | 3 | 182.905 | 188.209 | -0.613 | 1.00 70.60 | Y | 0 |
| ATOM | 2461 | 02 | SO4 | | 3 | 185.274 | 188.143 | 0.172 | 1.00 70.08 | Y | 0 |
| MOTA | 2462 | 03 | SO4 | | 3 | 183.925 | 186.181 | 0.170 | 1.00 69.68 | Y | 0 |
| ATOM ATOM | 2463 2464 | 04 | SO4 | | 3 1 | 184.641 179.030 | 187.119 185.642 | -1.915 -6.293 | 1.00 70.92 1.00 8.84 | Y W | 0 |
| ATOM | 2464 | | WAT | | 2 | | 179.202 | -8.444 | 1.00 16.79 | W | 0 |
| ATOM | 2466 | | WAT | | 3 | 192.921 | 180.168 | 8.084 | 1.00 30.46 | W | Ö |
| ATOM | 2467 | OH2 | WAT | W | 4 | | 175.656 | 4.804 | 1.00 16.00 | W | 0 |
| MOTA | 2468 | | WAT | | 5 | | 169.305 | -5.499 | 1.00 13.87 | W | 0 |
| ATOM | 2469 | | WAT | | 6 | | 180.066 | 22.244 | 1.00 15.19 | W | 0 |
| ATOM | 2470 | | WAT | | 7 8 | 180.414 | 171.384 | 22.814 | 1.00 8.30 1.00 10.24 | W | 0 |
| MOTA MOTA | 2471 2472 | OH2 | WAT | | | | 184.543 181.649 | -6.390 3.509 | 1.00 10.24 | W W | 0 |
| ATOM | 2473 | | WAT | | | | 157.114 | 14.496 | 1.00 16.39 | W | Ö |
| ATOM | 2474 | | WAT | | 11 | | 158.543 | 18.441 | 1.00 20.42 | W | 0 |
| ATOM | 2475 | | WAT | | | 194.144 | | 11.618 | 1.00 13.61 | W | 0 |
| MOTA | 2476 | | WAT | | | | 183.197 | -8.077 | 1.00 36.64 | . W | 0 |
| ATOM | 2477 | | WAT | | | | 147.344 170.073 | -7.377 -2.678 | 1.00 23.99 | . M | 0 |
| ATOM ATOM | 2478 2479 | | TAW | | | | 162.247 | 7.860 | 1.00 18.36 1.00 20.24 | W W | 0 |
| ATOM | 2480 | | WAT | | | | 175.122 | -2.821 | 1.00 12.41 | W | ŏ |
| ATOM | 2481 | | WAT | | 18 | | 168.406 | 2.165 | 1.00 9.98 | W | Ó |
| MOTA | 2482 | | WAT | | | | 176.594 | 9.704 | 1.00 27.47 | W | 0 |
| ATOM | 2483 | | WAT | | | 193.215 | | 11.973 | 1.00 17.15 | W | 0 |
| ATOM | 2484 2485 | | WAT WAT | | | 188.165 | 173.468 189.493 | 14.493 5.006 | 1.00 18.83 1.00 25.99 | W W | 0 |
| ATOM ATOM | 2485 | | WAT | | | 194.904 | 178.835 | 14.332 | 1.00 23.99 | W | 0 |
| MOTA | 2487 | | WAT | | | 172.594 | | 25.336 | 1.00 22.88 | W | Ö |
| MOTA | 2488 | OH2 | WAT | ' W | 25 | 186.612 | 173.366 | -9.877 | 1.00 19.22 | W | 0 |
| ATOM | 2489 | | WAT | | | | 183.702 | 20.193 | 1.00 22.57 | W | 0 |
| ATOM | 2490 | | WAT | | | | 160.388 | 11.646 | 1.00 15.90 | W | 0 |
| ATOM ATOM | 2491 2492 | | TAW TAW | | | | 174.788 186.952 | 11.702 32.619 | 1.00 18.10 1.00 32.00 | W W | 0 |
| ATOM | 2493 | | WAT | | | | 163.564 | | 1.00 32.00 | W | Ö |
| ATOM | 2494 | | WAT | | | | 165.930 | -0.838 | 1.00 16.37 | W | ŏ |
| ATOM | 2495 | | WAT | | | | 190.638 | 21.333 | 1.00 17.02 | W | 0 |
| MOTA | 2496 | | TAW | | | | 181.451 | 8.363 | 1.00 23.84 | W | 0 |
| ATOM | 2497 | | WAT | | | | 183.136 172.283 | 11.412 | 1.00 27.78 | W | 0 |
| ATOM ATOM | 2498 2499 | | raw raw | | | | 172.203 | 12.285 -8.556 | 1.00 22.44 1.00 14.47 | W W | 0 |
| ATOM | 2500 | OH2 | WAI | . W | 37 | | 178.975 | 16.555 | 1.00 28.73 | M | Ö |
| ATOM | 2501 | | WAT | | | | 191.015 | 5.492 | 1.00 22.39 | W | ŏ |
| ATOM | 2502 | | TAW | | | | 163.980 | -2.087 | 1.00 16.88 | W | 0 |
| ATOM | 2503 | | TAW | | | | 174.714 | 13.402 | 1.00 14.25 | W | 0 |
| ATOM | 2504 | | VAT | | | | 189.228 | 27.405 | 1.00 21.42 | W | 0 |
| ATOM ATOM | 2505 2506 | | TAW TAW | | | | 175.020 166.218 | 21.436 | 1.00 32.61 1.00 18.57 | W W | 0 |
| ATOM | 2507 | | WAI | | | | 150.396 | 10.582 | 1.00 18.37 | W | 0 |
| ATOM | 2508 | | WAT | | | | 183.843 | 1.498 | 1.00 23.82 | W | ő |
| MOTA | 2509 | | WAT | | | 203.088 | 159.272 | -4.093 | 1.00 20.75 | W | Ö |
| ATOM | 2510 | | WAT | | | | 190.097 | 18.980 | 1.00 22.00 | W | 0 |
| ATOM | 2511 | | WAT | | | | 164.352 | 18.292 | 1.00 18.52 | W | 0 |
| ATOM | 2512 | | VAT | | | | 192.170 188.073 | 8.139 29.292 | 1.00 29.33 1.00 22.03 | W | 0 |
| ATOM | 2513 | OH2 | WAT | W | 50 | 1/0.708 | 100.0/3 | 43.434 | 1.00 22.03 | M | 0 |

| | | | | | | | | | | | | _ |
|------|------|-----|--------------|---|-----|---------|-----------|---------|------|-------|---|-----|
| MOTA | 2514 | OH2 | WAT | W | 51 | 179.041 | 176.835 | -4.879 | 1.00 | 28.93 | W | 0 |
| MOTA | 2515 | OH2 | WAT | W | 52 | 177.094 | 169.275 | 14.745 | 1.00 | 17.83 | W | 0 |
| ATOM | 2516 | OH2 | | | 53 | 173.359 | 158.848 | 5.717 | 1.00 | 26.69 | W | 0 |
| | | | | | | | 145.517 | -1.099 | | 25.66 | W | ŏ |
| ATOM | 2517 | | WAT | | 54 | | | | _ | | | |
| MOTA | 2518 | | WAT | | 55 | | 162.673 | 24.709 | _ | 31.35 | W | 0 |
| MOTA | 2519 | OH2 | WAT | W | 56 | 190.279 | 149.132 | -0.366 | 1.00 | 23.37 | W | 0 |
| ATOM | 2520 | OH2 | WAT | W | 57 | 175.195 | 156.308 | 1.515 | 1.00 | 25.31 | W | 0 |
| ATOM | 2521 | | TAW | | 58 | 189.320 | 149.244 | 12.871 | 1.00 | 39.74 | W | 0 |
| | | | | | | | 160.562 | 17.366 | | 19.61 | W | Ö |
| MOTA | 2522 | | TAW | | 59 | | | | | | | |
| MOTA | 2523 | OH2 | WAT | W | 60 | | 189.438 | 10.191 | | 32.59 | W | 0 |
| ATOM | 2524 | OH2 | WAT | W | 61 | 176.96 | 195.154 | 23.343 | 1.00 | 26.84 | W | 0 |
| MOTA | 2525 | OH2 | TAW | W | 62 | 194.908 | 3 178.479 | 10.038 | 1.00 | 12.42 | W | 0 |
| ATOM | 2526 | | | W | 63 | 192.933 | 176.681 | 8.727 | 1.00 | 17.49 | W | 0 |
| | | | | | | | 178.650 | 10.287 | | 25.58 | W | Ö |
| ATOM | 2527 | | TAW | | 64 | | | | | | | |
| MOTA | 2528 | - | WAT | | 65 | | 183.023 | | | 15.88 | W | 0 |
| MOTA | 2529 | OH2 | war | W | 66 | 174.84 | 179.377 | 29.234 | | 21.85 | W | 0 |
| ATOM | 2530 | OH2 | TAW | W | 67 | 192.66 | 5 150.025 | 4.037 | 1.00 | 24.70 | W | 0 |
| ATOM | 2531 | OH2 | WAT | W | 68 | 191.22 | 7 167.117 | 19.848 | 1.00 | 27.52 | W | 0 |
| ATOM | 2532 | | WAT | | 69 | | 3 166.787 | -4.678 | | 16.05 | W | 0 |
| | | | | | | | | | | | W | ŏ |
| MOTA | 2533 | | WAT | | 70 | | 3 164.953 | 24.250 | | 16.65 | | |
| MOTA | 2534 | OH2 | \mathbf{v} | W | 71 | 202.92 | 1 187.953 | 5.807 | | 25.48 | W | 0 |
| MOTA | 2535 | OH2 | WAT | W | 72 | 173.65 | 6 180.838 | -1.296 | 1.00 | 19.16 | W | 0 |
| ATOM | 2536 | OH2 | WAT | W | 73 | 178.22 | 3 170.722 | 21.753 | 1.00 | 28.96 | W | 0 |
| ATOM | 2537 | | WAT | | 74 | | 7 185.273 | 4.691 | | 36.63 | W | 0 |
| | | | | | | | | | | 54.41 | W | ő |
| ATOM | 2538 | | WAT | | 75 | | 1 160.492 | 21.694 | | | | |
| MOTA | 2539 | OH2 | TAW | W | 76 | 174.34 | 3 151.575 | -4.090 | | 24.22 | W | 0 |
| MOTA | 2540 | OH2 | WAT | W | 77 | 199.21 | 7 156.232 | 8.084 | 1.00 | 24.50 | W | 0 |
| ATOM | 2541 | OH2 | WAT | W | 78 | 186.69 | 3 195.451 | 15.184 | 1.00 | 30.28 | W | 0 |
| ATOM | 2542 | OH2 | WAT | W | 79 | 204.07 | 2 167.051 | -16.474 | 1,00 | 30.81 | W | 0 |
| | 2543 | | WAT | | 80 | | 9 170.883 | 13.071 | | 24.00 | W | |
| MOTA | | | | | | | | | | | | |
| MOTA | 2544 | | WAT | | 81 | | 2 167.033 | 18.576 | | 34.40 | W | |
| ATOM | 2545 | OH2 | WAT | W | 82 | 188.05 | 5 177.150 | -16.174 | 1.00 | 39.31 | W | 0 |
| ATOM | 2546 | OH2 | WAT | W | 83 | 209.16 | 7 161.801 | -3.764 | 1.00 | 29.76 | W | 0 |
| MOTA | 2547 | OH2 | WAT | W | 84 | 189.95 | 4 187.203 | -3.104 | 1.00 | 30.21 | W | 0 |
| ATOM | 2548 | | WAT | | 85 | | 6 175.210 | 9.226 | | 35.64 | W | |
| | | | | | | | | | | 29.71 | W | |
| MOTA | 2549 | | WAT | | 86 | | 8 162.643 | | | | | |
| ATOM | 2550 | OH2 | WAT | W | 87 | | 3 164.861 | | | 23.03 | M | |
| ATOM | 2551 | OH2 | TAW | W | 88 | 176.98 | 5 177.272 | 13.711 | 1.00 | 28.39 | W | 0 |
| MOTA | 2552 | OH2 | WAT | W | 89 | 197.77 | 5 160.663 | 10.355 | 1.00 | 30.90 | W | 0 |
| ATOM | 2553 | OH2 | WAT | W | 90 | 180.41 | 8 156.423 | -15.983 | 1.00 | 38.69 | W | 0 |
| ATOM | 2554 | | WAT | | 91 | | 3 165.048 | | | 39.85 | W | |
| | | | | | | | 8 146.684 | | | 28.72 | W | |
| ATOM | 2555 | | WAT | | 92 | | | | | | | |
| MOTA | 2556 | OH2 | WAT | W | 93 | | 8 173.307 | | | 20.55 | W | |
| ATOM | 2557 | OH2 | WAT | W | 94 | 195.43 | 3 186.638 | 2.426 | 1.00 | 32.36 | W | 0 |
| MOTA | 2558 | OH2 | WAT | W | 95 | 185.68 | 9 149.073 | 10.194 | 1.00 | 32.44 | W | 0 |
| ATOM | 2559 | OH2 | WAT | W | 96 | 181.72 | 5 186.361 | 4.468 | 1.00 | 44.13 | W | 0 |
| | | OH2 | | | 97 | | 8 181.376 | | | 40.50 | W | |
| ATOM | 2560 | | | | | | 1 164.983 | | | | | |
| MOTA | 2561 | | TAW | | 98 | | | | | 30.78 | W | |
| MOTA | 2562 | | WAT | | 99 | | 0 148.459 | | | 29.87 | W | |
| ATOM | 2563 | OH2 | WAT | W | 100 | 172.18 | 6 178.856 | -0.480 | 1.00 | 35.57 | W | 0 |
| ATOM | 2564 | OH2 | WAT | W | 101 | 195.54 | 1 178.234 | 1.979 | 1.00 | 25.17 | W | . 0 |
| ATOM | 2565 | | WAT | | | 170.59 | 8 187.029 | 21.078 | 1.00 | 24.60 | W | 0 |
| | 2566 | | WAT | | | | 7 172.274 | | | 36.47 | W | |
| ATOM | | | | | | | | | | | | |
| ATOM | 2567 | | TAW | | | | 9 188.864 | | | 22.94 | W | |
| ATOM | 2568 | | WAT | | | | 0 190.812 | | | 32.99 | W | |
| ATOM | 2569 | OH2 | WAT | W | 106 | 201.81 | 6 192.555 | 4.023 | 1.00 | 28.31 | W | 0 |
| ATOM | 2570 | OH2 | WAT | W | 107 | 202.50 | 4 159.814 | -7.441 | 1.00 | 22.58 | W | 0 |
| ATOM | 2571 | | WAT | | | | 2 185.298 | | 1.00 | 31.96 | W | |
| | | | | | | | 7 179.403 | | | 39.35 | W | |
| ATOM | 2572 | | WAT | | | | | | | | | |
| MOTA | 2573 | | WAT | | | | 4 193.700 | | | 32.38 | W | |
| MOTA | 2574 | OH2 | WAT | W | 111 | 173.23 | 2 181.808 | -8.349 | 1.00 | 19.06 | W | 0 |
| ATOM | 2575 | OH2 | WAT | W | 112 | 182.82 | 7 187.517 | -4.364 | 1.00 | 45.61 | W | 0 |
| ATOM | 2576 | | WAT | | | | 8 194.231 | | | 42.16 | W | |
| | 2577 | | WAT | | | | 0 159.628 | | | 35.35 | w | |
| ATOM | | | | | | | | | | | | |
| ATOM | 2578 | | WAT | | | | 7 184.866 | | | 34.38 | W | |
| MOTA | 2579 | | TAW | | | | 2 197.288 | | | 39.58 | W | |
| ATOM | 2580 | OH2 | WAT | W | 117 | 199.84 | 1 150.695 | 13.176 | 1.00 | 35.40 | W | 0 |
| MOTA | 2581 | | WAT | | | | 6 180.622 | | 1.00 | 29.36 | W | 0 |
| ATOM | 2582 | | WAT | | | | 9 169.945 | | | 36.75 | W | |
| | | | | | | | 5 189.198 | | | 33.73 | W | |
| ATOM | 2583 | OH2 | WAT | W | 120 | 100.30 | O 102.130 | 21.310 | 1.00 | 55.13 | W | U |

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| ATOM | 2584 | он2 | WAT | W | 121 | 185.505 | 146.137 | -4.208 | 1.00 | 30.91 | W | 0 |
|------|------|-----|-----|---|-----|---------|-----------|---------|------|-------|----------|-----|
| ATOM | 2585 | OH2 | WAT | W | 122 | 168.783 | 176.131 | 0.277 | 1.00 | 37.59 | W | 0 |
| ATOM | 2586 | OH2 | WAT | W | 123 | 179.830 | 187.974 | 34.894 | 1.00 | 39.81 | W | 0 |
| ATOM | 2587 | OH2 | WAT | W | 124 | 194.391 | 191.022 | 26.003 | 1.00 | 35.26 | W | 0 |
| ATOM | 2588 | OH2 | WAT | W | 125 | 175.707 | 190.116 | 18.448 | 1.00 | 37.47 | M | 0 |
| MOTA | 2589 | OH2 | WAT | W | 126 | 172.799 | 187.052 | 31.328 | 1.00 | 38.58 | W | 0 |
| ATOM | 2590 | OH2 | WAT | W | 127 | 173.867 | 181.212 | 14.618 | 1.00 | 28.93 | W | 0 |
| ATOM | 2591 | OH2 | WAT | W | 128 | 169.850 | 183.554 | 9.734 | 1.00 | 31.19 | W | 0 |
| ATOM | 2592 | OH2 | WAT | W | 129 | 201.846 | 186.034 | 10.890 | 1.00 | 39.65 | W | 0 |
| ATOM | 2593 | OH2 | WAT | W | 130 | 192.263 | 183.101 | 8.973 | 1.00 | 35.20 | W | 0 |
| ATOM | 2594 | OH2 | WAT | W | 131 | 195.03 | 155.601 | 22.286 | 1.00 | 43.08 | W | 0 |
| ATOM | 2595 | OH2 | WAT | W | 132 | 188.13 | 149.463 | -10.689 | 1.00 | 31.69 | V | 0 |
| ATOM | 2596 | OH2 | WAT | W | 133 | 193.61 | 166.439 | 22.911 | 1.00 | 37.73 | ₩ | 0 |
| ATOM | 2597 | OH2 | WAT | W | 134 | 169.15 | 9 198.181 | -6.371 | 1.00 | 34.05 | W | 0 |
| ATOM | 2598 | OH2 | WAT | W | 135 | 173.143 | l 166.101 | 3.246 | 1.00 | 37.73 | V | 0 |
| ATOM | 2599 | OH2 | TAW | W | 136 | 196.413 | l 181.887 | 24.452 | 1.00 | 31.18 | V | 0 |
| ATOM | 2600 | OH2 | WAT | W | 137 | 166.87 | 5 190.046 | -8.389 | 1.00 | 35.44 | V | 1 0 |
| ATOM | 2601 | OH2 | WAT | W | 138 | 168.31 | 173.985 | 5.026 | 1.00 | 36.83 | V | 1 0 |
| ATOM | 2602 | OH2 | WAT | W | 139 | 191.55 | 3 162.337 | -15.173 | 1.00 | 30.34 | V | 1 0 |
| ATOM | 2603 | OH2 | WAT | W | 140 | 196.78 | 9 179.956 | 0.077 | 1.00 | 34.96 | V | 1 0 |
| MOTA | 2604 | OH2 | TAW | W | 141 | 204.36 | 2 177.082 | -3.998 | 1.00 | 42.74 | V | _ |
| ATOM | 2605 | OH2 | WAT | W | 142 | 178.23 | 7 157.118 | 15.427 | 1.00 | 37.51 | V | 1 0 |
| ATOM | 2606 | OH2 | WAT | W | 143 | 180.70 | 3 166.918 | | 1.00 | | V | |
| MOTA | 2607 | OH2 | WAT | W | 144 | 190.07 | 6 196.775 | 13.865 | 1.00 | 38.81 | V | 1 0 |